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MODIFIED DEACETOXYCEPHALOSPORIN C SYNTHASE (DAOCS) AND X-RAY STRUCTURE

Penicillin and cephalosporin antibiotics are produced either directly by fermentation or by modification of fermentation derived materials containing a beta-lactam ring. The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and reviewed (J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β -lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Ingolia and Queener, Med. Res. Rev., 1989, 9, 245-264; Aharonowitz, Cohen and Martin, Ann. Rev. Microbiol., 1992, 46, 461-495; Schofield, Bycroft, Baldwin, Hadju, Roach, Current Opinion in Structural Biology, 1997, 7, 857-864) and includes the following steps (Figure 1):

- Conversion of the tripeptide: \underline{L} - δ - α -aminoadipoyl- \underline{L} -cysteinyl-D-valine (ACV) to isopenicillin N in a step catalysed by isopenicillin N 15 synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
- In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its \underline{L} - δ - α -20 aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This conversion is catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be 25 commercially produced via fermentation under the appropriate conditions.
 - In other organisms (e.g. Streptomyces clavuligerus and Cephalosporium acremonium) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.

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- 4. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to DAOC. This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. C. acremonium).
- 5. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp.* DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins and their biosynthetic intermediates are useful as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins (including penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, *e.g.* Cefachlor.

The enzymes IPNS, DAOCS, DACS and DAOC/DACS are

members of an extended family of Fe(II) utilising oxidase and oxygenase
enzymes. Most of this family (including DAOCS, DACS and DAOC/DACS)
utilise a 2-oxo acid (normally 2-oxoglutarate) as a cosubstrate in addition to
dioxygen and the 'prime' substrate (e.g. penicillin N in the case of DAOCS).
Since IPNS, does not use 2-oxoglutarate, it has a substantially different
mechanism to the 2-oxoglutarate dependent oxygenases, and this gives

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rise to a significantly different active site.

The Invention

This invention is based on the determination of the three dimensional crystal structure of DAOCS and the information and developments which come from it. The X-ray co-ordinates provide very detailed 3-dimensional information on the relationships between amino acid residues in the structure of DAOCS and on the binding modes of the Fe-cofactor and the substrates to DAOCS. The structure allows the modification of DAOCS and related enzymes of penicillin and cephalosporin biosynthesis (including DACS and DAOC/DACS) in order to alter their substrate and product selectivities. Since the DAOCS structures are the first from the family of 2-oxoglutarate dependent dioxygenases they also allow for the design of new inhibitors of this family of enzymes. Previously partial overviews of the structures of IPNS complexed to manganese and IPNS complexed to iron and ACV were reported (Roach et al., Nature, 1995, 375, 700-704; Roach et al., Nature, 1997, 387, 827). The structures, as defined by their X-ray co-ordinates, of IPNS complexed to manganese and in complexes with iron, ACV and/or substrate analogues have been reported in Baldwin, Hajdu, Roach, Hensgens, Clifton, GB 9621486.1- (Oxygenase Enzymes and Method).

Procedures have been developed for the production of 7-aminodeacetoxycephaosporin C (7-ADCA) in which recombinant *P. chrysogenum* strains into which the DAOCS gene has been introduced are used for the production of cephalosporins. In particular if adipic acid is added to these recombinant strains adipoyl-6-APA is produced, which is converted by DAOCS into adipoyl-7-ADCA from which the adipoyl side chain can be removed (EPA-A-0532341, Shibata *et al.*, Bioorg. Med. Chem. Letts, 1996, 6, 1579-1584).

The IPNS gene sequence (and therefore the amino acid

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sequence) is related but significantly different to those of DAOCS, DACS, DAOC/DACS. It is likely that gross elements of the fold (i.e. significant elements within the 3-dimensional structure) of these enzymes will be conserved but that the active site architecture will be very significantly different. Structural elements conserved are likely to include the beta-barrel 'jelly roll' core and certain alpha-helices (including alpha helix-10, as defined in Roach et al., Nature, 1995, 375, 700-704). The degree of similarity is insufficient to define the precise structure of DAOCS, DACS, or DAOC/DACS from the IPNS structures. To date no models of DAOCS, DACS, or DAOC/DACS based on the IPNS structure have been reported. Nor have any detailed studies on substrate binding of these enzymes been reported. One report (WO 97/20053) claims the use of products resulting from modification of certain residues in DAOCS for the improved conversion of penicillin G to phenyl acetyl (G)-7-aminocephalosporanic

acid.

The three-dimensional structure of DAOCS is defined by the X-ray co-ordinates set out below (Structure A).

Also set out below is a high resolution crystal structure of a complex of prokaryotic DAOCS from *S. clavuligerus* with Fe(II) and 2-oxoglutarate (Structure B).

In part the present invention relates to the use of the structures of DAOCS in order to make modifications to it or DACS or DAOC/DACS in order that the modified enzymes catalyse the conversion of unnatural penicillins (e.g. penicillin G and penicillin V) to cephalosporins more efficiently than the wild-type enzyme. Further aspects of the invention relate to the use of the DAOCS structure in order to produce unnatural products in micro-organisms. Such products include exomethylene cephalosporins, with or without alpha-aminoadipoyl or hydrophobic side chain (e.g. phenylacetyl or phenoxyacetyl). Thus one aspect of this invention refers to the use of the structure of DAOCS for modifying DAOCS

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(or the closely related enzymes DACS or DAOC/DACS) in order to:

- (i) permit the enzyme to accept (or accept more efficiently) unnatural penicillin substrates for the preparation of new or commercially valuable antibacterial materials.
- (ii) enable the modified enzyme to produce unnatural (e.g. exomethylene cephams) or optimise the production of minor products (e.g. $3-\beta$ -hydroxycephams) for use as antibacterials or as intermediates in the preparation of antibacterials or commercially valuable compounds.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with DAOCS. Thus, structures of these enzymes may be predicted on the basis of the DAOCS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of DAOCS. Previous sequence comparisons (Roach et al., Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the structure of one enzyme (e.g. DACS or DAOC/DACS) from another closely related enzyme (e.g. DAOCS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are

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largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary structural elements. The effect of these differences, which alter the substrate/product selectivities of the compared enzymes, is predictable once the three-dimensional structure of one of the enzymes is known.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the side chain binding site of penicillin N or DAOC is modified and at at least one of the following sites at least one amino acid residue is changed to another amino acid residue or is deleted: Thr72, Arg74, Arg75, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Modifications of this kind will permit the expansion of penicillin V or penicillin G to the corresponding cephalosporins. To achieve this it is desirable to increase the kcat/Km for the mutant as compared to the wild type DAOCS. Kinetic results indicate that apparent kcat values for penicillin N and penicillin G are similar but that Km is much higher for penicillin G. Thus based on these analysis, a decrease in the binding constant of DAOCS for penicillin G should make it possible to increase kcat/Km for penicillin G.

The side chain binding pocket of DAOCS is made of residues from different parts of the peptide chain, so it is likely that more than one residue will have to be altered to make a better penicillin G/V expander. Nevertheless some residues are more important than others. Examination of the interactions between the last few C-terminal residues (Thr-308 to Ala-311) of one DAOCS molecule and the active site of another in the crystal structure, suggests a binding mode for the penicillin nucleus which

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is shown in Figure 2 of the accompanying drawings. The penam C-3 carboxylate group probably occupies an analogous position to that of Ala-311 from a symmetry related molecule in the active site, forming electrostatic interactions with Arg-162 and Arg-160. The side chain of Arg-160 may also form a hydrogen bonding interaction with the β -lactam carbonyl.

It needs to be borne in mind that protein specificity is generally controlled by more than one amino acid. To alter the specificity of a protein in a major way is likely to require more than one of the mutational changes suggested below, although each of the mutations will contribute. With this in mind, preferred residues to modify for the expansion of a penicillin are as follows:

- a) Arg-266. This residue binds with the α -aminoadipate side chain of the natural substrate and should be changed to a residue of more hydrophobic character, e.g. Phe, Ala, Val, Leu, Ile.
- b) Thr-72. This should be changed to a hydrophobic residue e.g. Val, Leu, Ile, Phe, Ala, to help bind the hydrophobic side chain of penicillin G. It should be effective in combination with other mutants.
- c) Arg-74 may be usefully changed to a neutral or hydrophobic residue (Phe, Tyr, Val, Leu, Ile, Ala). Modification of Arg-75 may be necessary in addition because it forms a hydrogen-bonding network with Arg-74.
- d) Glu-156. This residue binds with the α -aminoadipate side chain. It should be changed to one of Ala, Val, Leu, Ile, Phe, Tyr, Trp, Asn, Gln, Ser.
- e) The side chains of Leu-158, Asn-301 and Tyr-302 form part of the binding pocket for the penicillin side chain and can be usefully modified to more hydrophobic character.
 - f) Asn-304. This residue binds the amide linking the side chain to the penam nucleus. Modification is effected to expand penicillins with shortened or no side chains (e.g. to Asp or Glu for 6-Apa).

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Note that other changes may be used to construct part or all of a side chain binding pocket via hydrogen bonding or other interactions.

The insertion or deletion of residues into the DAOCS sequence may also be of use in constructing a hydrophobic binding pocket for the penicillin side chain. Insertion of hydrophobic residues into the C-terminal region (residue 300-311 and in particular 301-303) may assist in the construction of a hydrophobic binding pocket for penicillin side chains.

In another aspect the invention provides an enzyme having significant (as herein defined) sequence similarity to DAOCS wherein the penicillin/cephalosporin binding site of penicillin N or DAOC is modified and at at least one of the following amino acid residues is changed or deleted: Ile88, Arg160, Arg162, Phe164, Met180, Thr190, Ile192, Phe225, Pro241, Val245, Val262, Phe264, Asn304, Ile305, Arg306, Arg307; and/or at least one additional amino acid residue is inserted within the region 300-311; provided that other residues interacting with the above may be changed in order to accommodate the change in one of the above.

Further discussion of this aspect may be found in Nature Volume 394, pages 805-809 published on 20 August 1998 and incorporated by reference herein.

Another aspect of the invention refers to the use of the structure of DAOCS in order to modify its active site (or that of a structurally related 2-oxoglutarate dependent dioxygenase) in order that the modified enzyme accepts non beta lactam substrates in order to produce oxidised compounds of value. Oxidised amino acids (e.g. 4-hydroxyprolines, hydroxylysines, hydroxyaspartic acids and others) are useful as synthetic intermediates in the production of valuable materials. Using the structure of DAOCS specific residues can be targeted for modification in order that the modified enzyme can be used to produce oxidised amino acids or peptides. The process may include modification of the following residues:

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Arg74, Glu156, Leu158, Arg160, Arg162, Leu186, Ser187, Phe225, Phe264, Arg266, Asp301, Tyr302, Val303, Asn304, Ile88, Arg162, Phe164, Met180, Thr190, Ile192, Pro241, Val245, Val262, Ile305, Arg306, Arg307.

Another aspect of the invention refers to the use of the DAOCS structure for the design of selective inhibitors of 2-oxoglutarate dependent dioxygenases. The 2-oxoglutarate dependent dioxygenase prolyl 4-hydroxylase has been the target of inhibition in order to provide a therapeutic treatment for fibrotic diseases (e.g. liver cirrhosis, arthritis). However, no inhibitors are in clinical use, probably because it is difficult to achieve selective inhibition of the target enzyme for inhibition over other enzymes (including 2-oxoglutarate dependent enzymes). The structure of DAOCS provides a template for the design of inhibitors of 2-oxoglutarate dependent dioxygenases.

Set out below are two high resolution crystal structures for DAOCS from *S. clavuligerus*: the structure of the iron-free apoenzyme (Structure A) and the structure of the complex with Fe(II) and 2-oxoglutarate (Structure B). The results imply a mechanism by which the enzyme-Fe(II) complex reacts with 2-oxoglutarate and dioxygen to give the reactive ferryl species, a process common to many non-haem oxygenases. Other notable 2-oxoacid-dependent ferrous enzymes are prolyl hydroxylase, involved in collagen biosynthesis, gibberellin 3β-hydroxylase, a mutation of which influences stem length in plants, and clavaminic acid synthase, involved in the biosynthesis of the β-tactamase inhibitor, clavulanic acid. Within the family of 2-oxoacid-dependent enzymes, DAOCS belongs to a sub-family, the members of which show sequence similarity with IPNS and 1-aminocyclopropane-1-carboxylate oxidase (the ethylene forming enzyme), enzymes that do not use a 2-oxoacid in catalysis.

The iron-free form of DAOCS crystallises in space group R3

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as a crystallographic trimer. The main chain of the protein folds into a conserved jelly roll core with flanking helices.

Co-ordinates and structure factors have been deposited with the Protein Data Bank (entries 1rxg, and r1rxgsf for the Fe(II)-2-oxoglutarate complex).

LEGENDS TO FIGURES.

Figure 1: the biosynthetic pathway to the penicillins and cephalosporins.

Figure 2 is a view of the active site of DAOCS showing 2-oxoglutarate binding to the iron and proposed penicillin N binding. Interactions with the side chains of certain amino acid residues are indicated by arrows.

Structure A is a three-dimensional structure of DAOCS.

Structure B is a high resolution crystal structure for prokaryotic DAOCS from *S. clavuligerus* as a complex with Fe(II) and 2-oxoglutarate.

The peptide sequence of DAOCS (with the numbering used herein) is set out below:

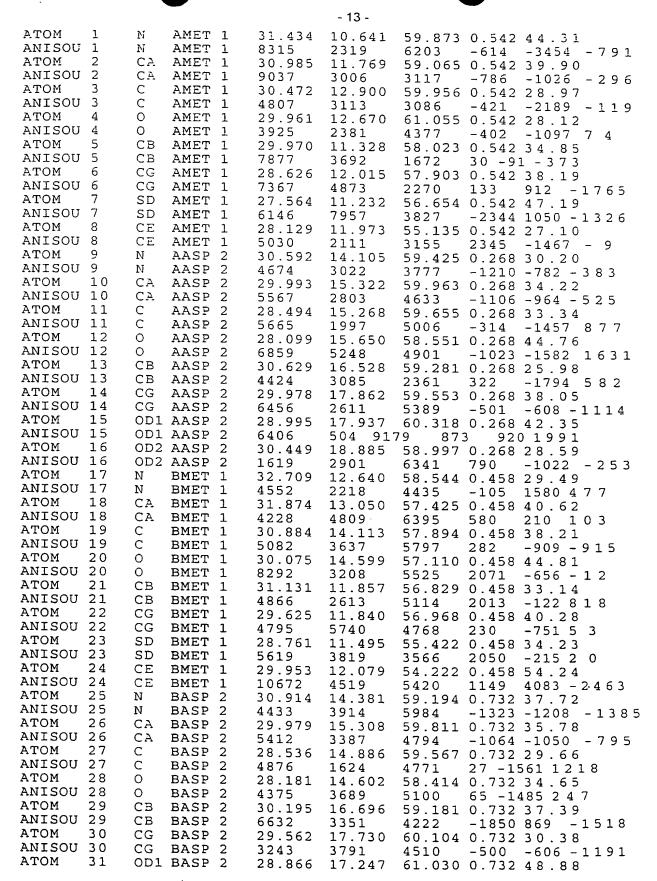
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	Glu	Phe	Arg	Arg	Cys	Leu	Arg	Asp	Lys	Gly	30
	Leu	Phe	Tyr	Leu	Thr	Asp	Cys	Gly	Leu	Thr	40
5	Asp	Thr	Glu	Leu	Lys	Ser	Ala	Lys	Asp	Leu	50
	Val	Ile	Asp	Phe	Phe	Glu	His	Gly	Ser	Glu	60
	Ala	Glu	Lys	Arg	Ala	Val	Thr	Ser	Pro	Val	70
	Pro	Thr	Met	Arg	Arg	Gly	Phe	Thr	Gly	Leu	80
	Glu	Ser	Glu	Ser	Thr	Ala	Gln	Ile	Thr	Asn	90
10	Thr	Gly	Ser	Tyr	Ser	Asp	Tyr	Ser	Met	Cys	100
	Tyr	Ser	Met	Gly	Thr	Ala	Asp	Asn	Leu	Phe	110
	Pro	Ser	Gly	Asp	Phe	Gly	Arg	Ile	Trp	Thr	120
	Gln	Tyr	Phe	Asp	Arg	Gln	Tyr	Thr	Ala	Ser	130
	Arg	Ala	Val	Ala	Arg	Glu	Val	Leu	Arg	Ala	140
15	Thr	Gly	Thr	Glu	Pro	Asp	Gly	Gly	Val	Glu	150
	Ala	Phe	Leu	Asp	Cys	Glu	Pro	Leu	Leu	Arg	160
	Phe	Arg	Tyr	Phe	Pro	Gln	Val	Pro	Glu	His	170
	Arg	Ser	Ala	Glu	Glu	Gln	Pro	Leu	Arg	Met	180
	Ala	Pro	His	Tyr	Asp	Leu	Ser	Met	Val	Thr	190
20	Leu	Ile	Gln	Gln	Thr	Pro	Cys	Ala	Asn	Gly	200
	Phe	Val	Ser	Leu	Gln	Ala	Glu	Val	Gly	Gly	210
	Ala	Phe	Thr	Asp	Leu	Pro	Tyr	Arg	Pro	Asp	220
	Ala	Val	Leu	Val	Phe	Cys	Gly	Ala	Ile	Ala	230
	Thr	Leu	Val	Thr	Gly	Gly	Gln	Val	Lys	Ala	· 240
25	Pro	Arg	His	His	Val	Ala	Ala	Pro	Arg	Arg	250
	Asp	Gln	Ile	Ala	Gly	Ser	Ser	Arg	Thr	Ser	260
	Ser	Val	Phe	Phe	Leu	Arg	Pro	Asn	Ala	Asp	270
	Phe	Thr	Phe	Ser	Val	Pro	Leu	Ala	Arg	Glu	280
	Cys	Gly	Phe	Asp	Val	Ser	Leu	Asp	Gly	Glu	290
30	Thr	Ala	Thr	Phe	Gln	Asp	Trp	Ile	Gly	Gly	300
	Asn	Tyr	Val	Asn	Ile	Arg	Arg	Thr	Ser	Lys	310
	Ala										311
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STRUCTURE A

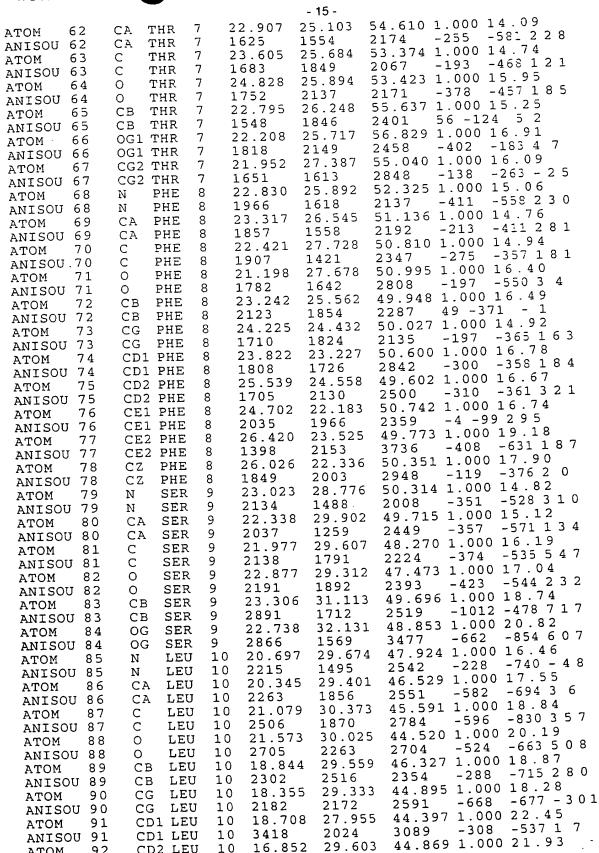


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ANISOU 33	N THR 3	4586 4123	4811 601 -1628 1516 60.495 1.000 40.48
ATOM 34	CA THR 3	26.303 14.433 4650 4555	6175 371 -911 -385
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ATOM 35 ANISOU 35	C THR 3	4376 4155	6598 320 -3864 -586 60.751 1.000 33.55
ATOM 36	O THR 3	24.150 15.556 4668 3107	4972 357 -2748 -588
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ATOM 38	OG1 THR 3	26.591 13.851	62.817 1.000 61.83 7476 -4164 -3020 2051
ANISOU 38	OG1 THR 3	10134 5882 26.399 12.052	61 278 1.000 59.32
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ATOM 41	CA THR 4	25.439 18.092 4275 4229	3358 -81 -1179 9 5
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ATOM 42 ANISOU 42	C THR 4	4876 3341	3207
ATOM 43	O THR 4	25.195 17.935 4877 3780	3363 1935 -1255 - 54
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ATOM 45	OG1 THR 4	27.324 19.09	1 61.578 1.000 32.36 4635 -79 -797 - 389
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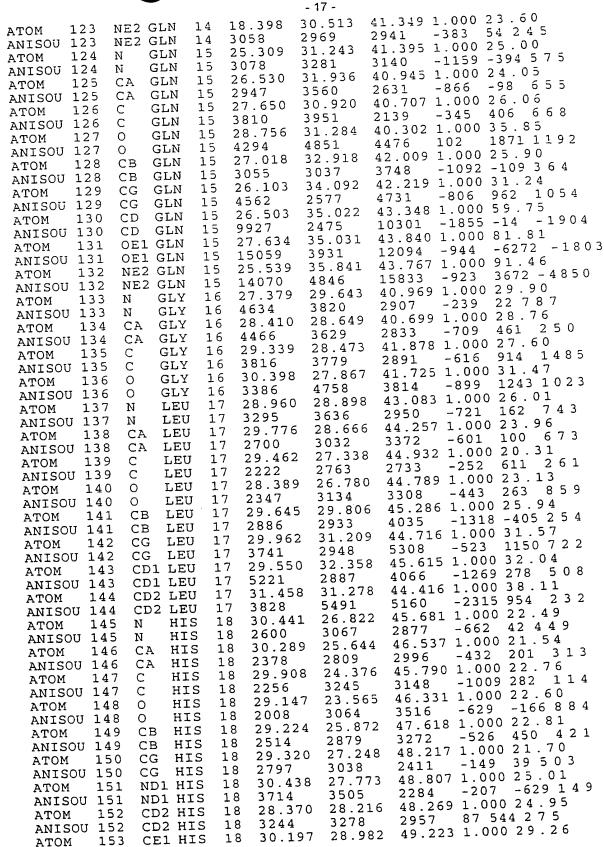
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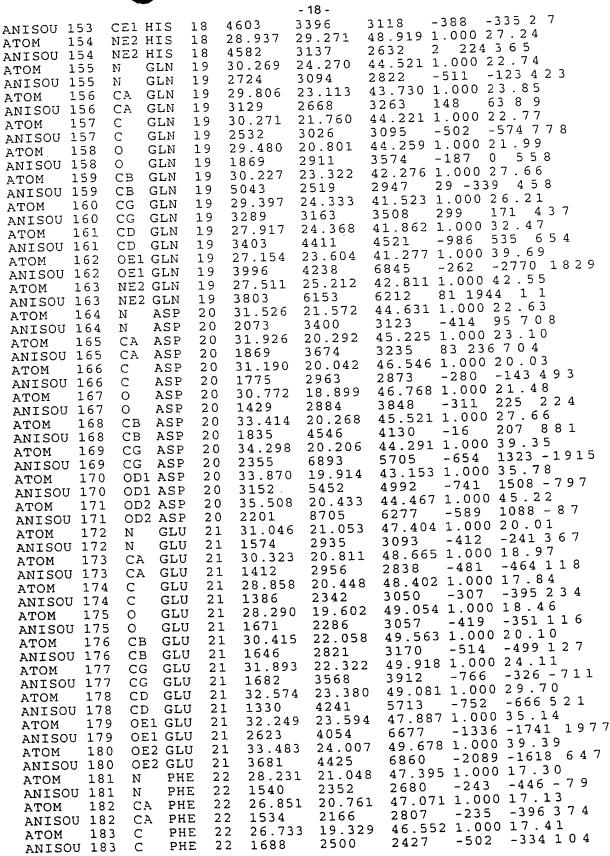
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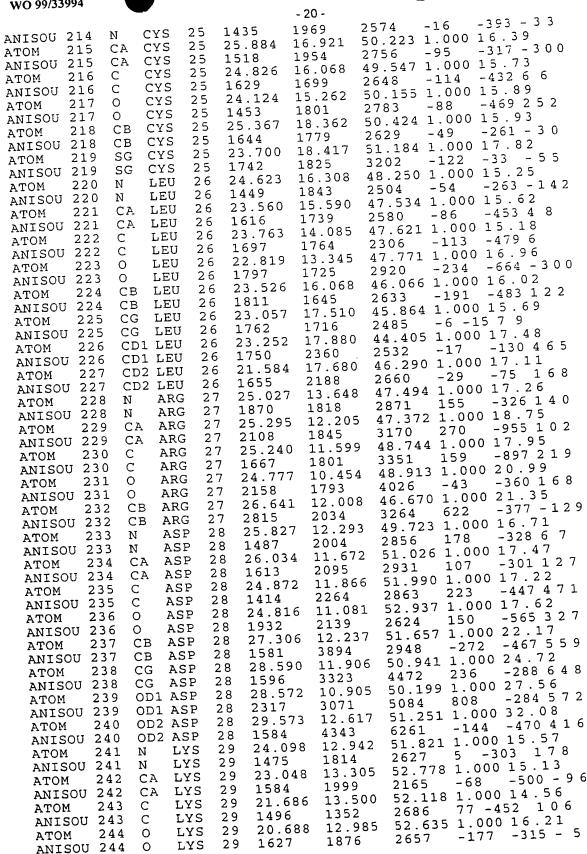
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ANISOU 11 ATOM 11 ANISOU 11 ATOM 11 ANISOU 11 ATOM 11	N ALA N ALA CA ALA CA ALA CA ALA CC A	13 2982 13 23.7 13 2313 13 22.5 13 2769 13 2709 1 13 2709 1 14 23.5 1 14 3596 1 14 23.2 1 14 3010	1975 31.463 2400 30.277 2179 30.215 2917 2192 31.170 2192 32.451 2316 7 32.279 2542 8 31.149 2681 9 2681 9 2681 9 2681 7 2347 2 28.566 2 29.295 2 345 1 27.137 2 28.566 2 32.45 2 28.095 3 216 2 28.095 3 216 2 28.095 3 216 2 28.095 3 216 2 28.095 3 216 2 29.295 4 2322 2 25.480 2 266 2 27.137 2 229 4 2332 2 25.480 2 266 2 3 27.137 2 2139 2 29.50 2 2139 8 29.97 3 335	45.953 1.000 3797 -461 46.005 1.000 3044 -828 45.862 1.000 2615 -506 44.920 1.000 2117 -702 44.069 1.000 2117 -1144 47.204 1.000 2636 -221 48.032 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2598 -344 49.389 1.000 2149 -1290 42.738 1.000 2275 -351 44.174 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 2149 -209 42.738 1.000 23845 -786 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 45.860 1.000 2422 -466 46.070 1.000 2845 -786 45.858 1.000 2635 -96	-1279 4 7 2 24 . 24 -979 8 9 1 21 . 06 -1016 4 3 1 26 . 29 -923 1 1 3 7 24 . 29 -216 9 9 6 20 . 65 -930 6 7 4 21 . 19 -715 5 9 8 21 . 56 -206 9 8 8 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 98 21 . 86 20 . 27 -624 5 0 1 20 . 54 -516 4 0 6 21 . 86 7 -612 7 9 9 02 4 . 98 8 -1088 1 1 3 4 03 3 . 5 2 9 -2251 4 6 018 . 91 -390 3 8 2 018 . 61 270 4 0 6 021 . 40 021 . 40 021 . 40 021 . 40 021 . 40 021 . 40 03 3 . 75 00 18 . 97 00 18 . 97 00 18 . 57 00 20 . 74 00 19 . 80 01 9 . 80
ATOM 11 ANISOU 11 ATOM 11 ANISOU 11 ATOM 11 ANISOU 11	3 CD1 LEU 3 CD1 LEU 4 CD2 LEU 4 CD2 LEU 5 N GLN 5 N GLN 6 CA GLN 6 CA GLN 7 C GLN 7 C GLN 8 O GLN	13 22.52 13 2769 13 25.02 13 2709 14 23.5 14 3596 14 3010 14 24.4 14 3360 14 24.4 11 3360 11 24.6	26 25.480 2266 23 25.47 2229 44 29.50 2139 84 29.97 3335 81 30.71 3427 55 30.82 4657	2845 -785 3 45.858 1.06 2585 -24 8 42.478 1.0 2635 -96 8 41.104 1.0 2694 -99 2 40.509 1.0 2881 -10 9 39.288 1.0 2922 -12	9 -142 5 9 4 00 19 . 8 0 4 -509 - 1 0 7 00 22 . 0 3 0 -903 3 7 9 00 23 . 7 9 2 -816 6 4 8 00 25 . 4 4 70 -382 4 8 7 00 30 . 0 4 08 -427 8 9 8
ATOM 11 ANISOU 11 ATOM 12 ANISOU 12 ATOM 13 ANISOU 13	19 CB GLI 19 CB GLI 20 CG GLI 20 CG GLI 21 CD GLI 21 CD GLI 22 OE1 GL	N 14 22.0 N 14 3133 N 14 20.7 N 14 3106 N 14 19.5 N 14 3386 N 14 19.5	30.90 3630 772 30.11 5 2319 586 31.02 4 2462 734 32.10	3222 -76 .1 41.355 1.0 3413 -29 20 41.631 1.0 3155 -33	-863 9 3 6 -863 9 3 6 -863 9 3 6 -863 9 3 6 -99 -577 5 1 4 -900 23 . 69 -17 -393 - 1 9 6 -17 -393 - 1 9 6 -17 -393 - 1 9 6

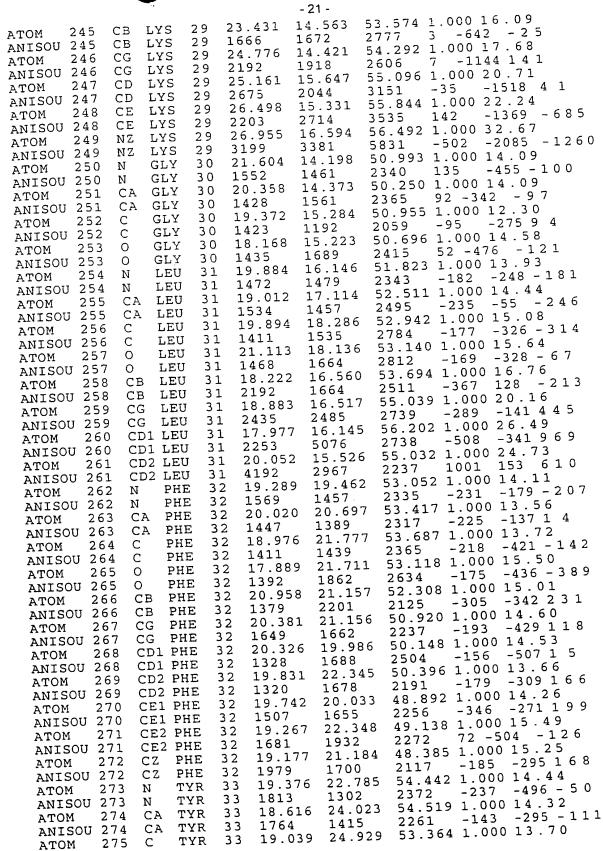


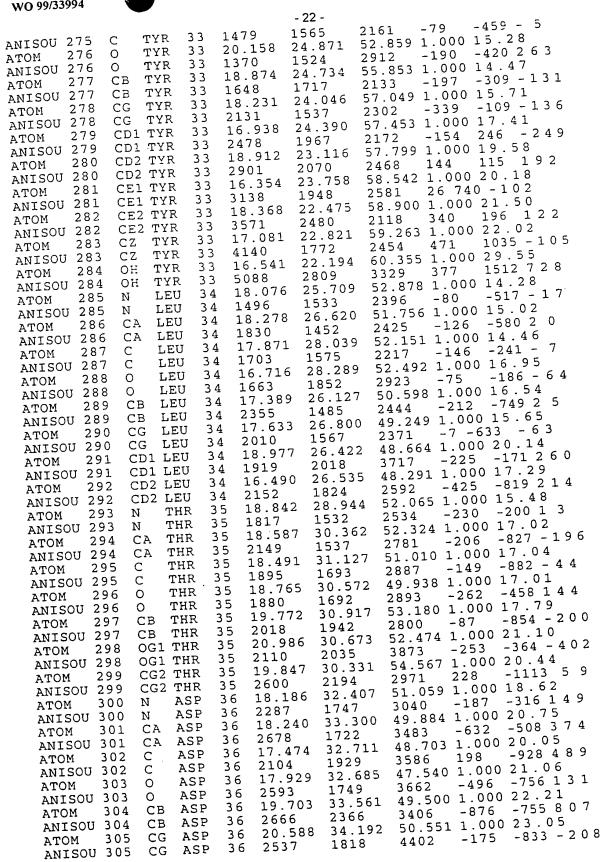


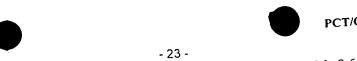


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104 0	PHE 22		8.574	46.995 1.000 15.87
ATOM 184 O	PHE 22		110	2343 -249 -361 1 3 1
MINIBOO			1.840	46.149 1.000 18.00
ATOM 185 CE ANISOU 185 CE		1747 2		2337 70 -178 4 4 5
ATOM 186 CG				45.930 1.000 16.38 2714 -90 -326 2 2 3
ANISOU 186 CO	PHE 22			2714 -90 -326 2 2 3 47.003 1.000 18.29
атом 187 CI	1 PHE 22		21.723	
ANTSOU 187 CI	1 PHE 22		2091 21.720	3045 -197 -88 5 / 6 44.641 1.000 18.62
ATOM 188 CI	02 PHE 22	24.290 2 2106 2	21.720	2890 -143 -623 3 9 4
	02 PHE 22 E1 PHE 22	22.569	21.727	46.771 1.000 18.90
	E1 PHE 22 E1 PHE 22		2086	3271 -198 -133 3 0 2
1111, 200	E2 PHE 22		21.660	44.379 1.000 19.28
ATOM 190 C. ANISOU 190 C	E2 PHE 22	2189	2023	3114 -242 -754 - 144
ATOM 191 C		22.059	21.645	45.473 1.000 19.42 3607 90 -483 -376
ANISOU 191 C	Z PHE 22		1723	3607 90 -483 -376 45.583 1.000 17.88
ATOM 192 N	ARG 23		18.971	2709 -168 -218 3 1 7
ANISOU 192 N			2437 17.594	45.079 1.000 19.18
ATOM 193 C	A ARG 23		2539	3022 -166 36 158
1111	A ARG 23 ARG 23		16.595	46 211 1 000 19.11
ATOM 194 C			2461	3518 -173 -113 4 5 5
			15.547	46.229 1.000 18.82
ATOM 195 C ANISOU 195 C			2156	3381 -33 181 -128
ATOM 196	B ARG 2	3 28.605	17.351	44.030 1.000 22.81 2633 -34 -105 - 354
	B ARG 2		4099	2633 -34 -105 - 35 4 42.617 1.000 24.82
ATOM 197 (G ARG 2		17.790 4078	2752 191 -122 - 204
ALVIDOG	CG ARG 2		17.272	41 685 1.000 29.71
	D ARG 2 D ARG 2		5619	3168 -285 908 / 04
	CD ARG 2 NE ARG 2		18.206	
	NE ARG 2		5034	3851 -43 286 297
ATOM 200		3 30.549	19.360	41.148 1.000 29.49 3529 -225 606 177
ANTSOU 200	CZ ARG 2	3 2612	5063	3323
ATOM 201		3 29.536	19.665 4951	2923 -960 331 545
		3 3242 3 31.629	20.092	41 345 1,000 32.61
		3 31.629 3 2320	5347	4722 -134 519 ± / 9
		28.708	16.851	47.125 1.000 17.80
111011		4 1262	2168	3332 183 38 9 8
ATOM 204		24 28.930	15.899	48.222 1.000 18.85 3287 69 -162 105
ANTSOU 204		24 1368	2509	40 114 1 000 17.51
ATOM 205		24 27.701	15.811 2015	3181 132 -177243
ANISOU 205		24 1456 24 27.333		2 49 544 1 000 17 9 3
ATOM 206		24 27.333 24 1851	1965	2997 -16 -402 2 5 3
ANISOU 206 ATOM 207		24 30.203		1 48.991 1.000 19.88
ATOM 207 ANISOU 207		24 1685	2700	3169 -398 -218 4 4
ATOM 208		24 31.459	16.05	3 48.135 1.000 29.07 4954 269 203 7 0 9
ANISOU 208	CG ARG	24 1467	4625	49 016 1 000 41 . 84
ATOM 209	CD ARG	24 32.700	16.20 7021	7130 -451 -494 - 922
ANISOU 209	CD ARG	24 1745 24 33.690		2 40 464 1 000 57.06
ATOM 210	NE ARG NE ARG	24 33.690 24 4362	9316	gnna -3326 -669 -1141
ANISOU 210 ATOM 211	NE ARG CZ ARG	24 34.032	2 18.32	27 48.810 1.000 60.67
ATOM 211 ANISOU 211	CZ ARG	24 5961	10369	$\frac{6723}{6723} - \frac{4627}{6723} - \frac{1324}{6723} - \frac{1300}{6723}$
ATOM 212	NH1 ARG	24 33.43	0 18.98	30 49.799 1.000 49.70 4569 -951 -2185 2226
ANISOU 212	NH1 ARG	24 7748	6565	71 40 159 1 000 54 . 12
ATOM 213	NH2 ARG	24 34.99	7 18.9° 8490	3378 -3780 -2352 1007
ANISOU 213	NH2 ARG	24 8696 25 27.09		
ATOM 214	N CYS	25 21.05		



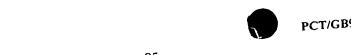


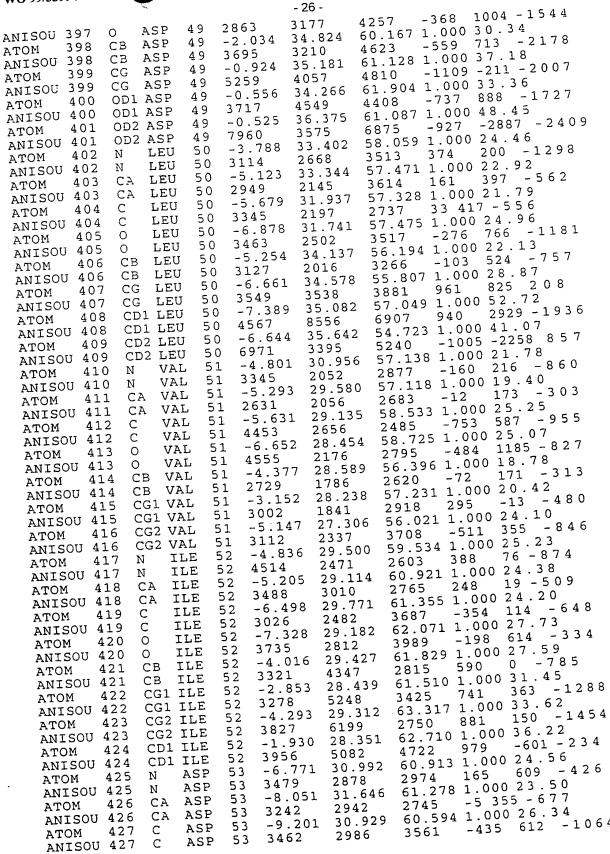






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ATOM 428 O ASP 53 -10.342 30.836 61.051 1.000 29.73 ANTSOU 428 O ASP 53 3468 3085 4743 -436 937 1.142 ANTSOU 429 C ASP 53 3468 3085 4767 -92 1806 937 ATOM 429 C ASP 53 3800 60.772 1.000 33.83 ATOM 430 C ASP 53 380.03 2322 6730 -92 1806 933 ATOM 430 C ASP 53 -9.038 33.758 60.583 1.000 32.05 1.38 ATOM 431 C DI ASP 53 -9.653 34.524 61.486 1.000 43.68 ATOM 431 C DI ASP 53 -9.653 34.524 61.486 1.000 43.76 8 ATOM 432 C DI ASP 53 -9.950 33.565 59.532 1.000 13.79 -312.0 ATOM 432 DI ASP 53 -9.950 33.565 59.532 1.000 13.79 -312.0 ATOM 432 DI ASP 53 -9.950 33.565 59.532 1.000 13.79 -312.0 ATOM 432 DI ASP 53 -9.950 33.376 59.413 1.000 25.39 ATOM 433 N PHE 54 -8.933 30.376 59.413 1.000 24.10 ATOM 434 C A PHE 54 -9.917 29.557 58.704 1.000 24.10 ATOM 435 C PHE 54 -0.180 28.259 59.486 1.000 24.00 ATOM 436 O PHE 54 -11.333 27.893 55.660 3.55 459 -68 8 ATOM 437 C B PHE 54 -9.465 29.273 57.260 1.355 459 -68 8 ATOM 438 C PHE 54 -9.465 29.273 57.261 1.000 24.10 ATOM 438 C PHE 54 -9.465 29.273 57.261 1.000 23.62 ATOM 439 C DI PHE 54 -11.333 27.893 55.666 1.000 24.00 ATOM 438 C PHE 54 -9.465 29.273 57.263 1.000 23.62 ATOM 439 C DI PHE 54 -11.733 27.893 55.666 1.000 24.00 ATOM 439 C DI PHE 54 -11.733 27.893 55.666 1.000 24.00 ATOM 439 C DI PHE 54 -11.733 27.893 55.666 1.000 24.00 ATOM 439 C DI PHE 54 -11.733 27.893 55.666 1.000 24.00 ATOM 430 C DI PHE 54 -11.729 29.078 56.087 1.000 23.62 ATOM 439 C DI PHE 54 -11.729 29.078 56.087 1.000 23.62 ATOM 439 C DI PHE 54 -11.729 29.078 56.087 1.000 23.62 ATOM 430 C DI PHE 54 -11.729 29.078 56.087 1.000 31.38 ATOM 430 C DI PHE 54 -12.265 28.499 56.461 1.000 27.62 1.000 42.23 ATOM 440 C D 2 PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.23 ATOM 440 C D 2 PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.33 ATOM 440 C D PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.33 ATOM 440 C D PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.33 ATOM 440 C D PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.33 ATOM 440 C D PHE 54 -50.522 84.99 56.461 1.000 27.62 1.000 42.33 ATOM 440 C D PHE 54 -50.522 84.90	WO 99/33994		•
ATOM 428 0 ASP 3 3468 3085 4743 -436 93 1122 ANISOU 429 CB ASP 53 -7964 33.084 60.772 1.000 33.83 -91122 ANISOU 429 CB ASP 53 -8062 2322 6730 -92 1806 -933 ANISOU 429 CB ASP 53 -8062 2412 5113 172 -302 -1138 ANISOU 430 CG ASP 53 -8652 2412 5113 172 -302 -1138 ANISOU 430 CG ASP 53 -8652 2412 5113 172 -302 -1138 ANISOU 431 ODI ASP 53 -8653 34.524 61.486 1.000 43.68 120 ATOM 431 ODI ASP 53 -8661 4686 248 150 1379 -3120 ANISOU 432 OD2 ASP 53 -9950 33.556 59.532 1.000 25.39 ATOM 432 OD2 ASP 53 -9950 33.556 59.532 1.000 25.39 ATOM 433 N PHE 54 -8933 30.376 59.413 1.000 25.39 ATOM 436 CA PHE 54 -9917 29.557 56.704 1.000 24.10 5.39 ANISOU 437 CB PHE 54 -311.333 27.89 59.686 1.000 24.10 68 8 ANISOU 436 O PHE 54 -3264 3174 2680 -366 263 -53 9 ANISOU 437 CB PHE 54 -11.332 27.89 59.686 1.000 24.00 68 8 ANISOU 437 CB PHE 54 -712 2945 2838 -694 -636 1 4 ANISOU 439 CDI PHE 54 -11.0522 28.499 56.46f 1.000 23.62 4 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 4 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 1 ANISOU 443 CR PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 1 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 1 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 1 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 62 1 ANISOU 440 CD2 PHE 54 -11.0522 28.499 56.46f 1.000 23.62 62 1 ANISOU 440 CD2 PHE 54 -12.653 28.406 551.307 1.000 42.33 8.4 ANISOU 440 CD2 PHE 54 -591.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 54 -591.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 54 -591.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 54 -591.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 54 -591.02 63.306 1.000 25.46 9.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 ANISOU 440 CD2 PHE 55 -501.02 63.306 1.000 38.69 8.7 A	•	₹.	- 27 -
ATOM 458 0 020 00	ATOM 428 ANISOU 428 ATOM 429 ANISOU 429 ATOM 430 ANISOU 431 ATOM 431 ATOM 432 ANISOU 433 ANISOU 433 ATOM 434 ANISOU 435 ATOM 435 ANISOU 436 ATOM 437 ANISOU 437 ANISOU 437 ANISOU 437 ANISOU 438 ATOM 438 ANISOU 438 ATOM 438 ANISOU 448 ANISOU 44	ASSPPPPPPEEEE OOCCOCCCCCCCCCCCCCCCCCCCCCCC	3 3468 33.084 6743 -436 9.37 142 33.084 67.79 1.000 33.83 33 3800 2322 6730 -92 18066 -933 3800 2322 6730 -92 18066 -933 3656 34652 2412 5113 172 -302 -1138 653 -9.563 34.524 61.486 1.000 43.68 13.79 -312 0 533 -9.653 34.524 61.486 1.000 43.68 13.79 -312 0 533 -9.950 33.556 59.532 1.000 51.30 2 53

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	O GLU 56	3864 8872 4150 35.85
ANISOU 458	CB GLU 56	-9.400
ATOM 459 ANISOU 459	CB GLU 56	503/ 5109 = 51401 1 000 38.63
ATOM 460	CG GLU 56	0.422
ANISOU 460	CG GLU 56	480 205 22 699 65.916 1.000 45.55
ATOM 461	CD GLU 56	-7.555 -255 -255
ANISOU 461	CD GLU 56 OF1 GLU 56	7 935 30.828 65.888 1.000 35.3 30.59
ATOM 462		7344 7247 6512 586 2370
ANISOU 462	OE1 GLU 56 OE2 GLU 56	-6 246 29 492 66 350 1 666 1163 - 2063
ATOM 463	OE2 GLU 56	4050 10497 4606 1 000 32.20
ANISOU 463	N HIS 57	4261 -549 1340 -070
ATOM 464 ANISOU 464	$_{ m N}$ HIS 57	32/3 4700 78 62,909 1.000 33.38
ATOM 465	CA HIS 57	1000 -110 1553 -1233
ANISOU 465		13 981 29 873 61.697 1.000 32.83
атом 466		1 -13.504 1 1200 - 17.5
ANISOU 466	,	7 - 15.012 30.533 61.571 276 1087 - 2205
ATOM 467		7 3362 4733 5990 7 1000 37 39
ANISOU 46		1 -12.002 -193 1402 -194
ATOM 468 ANISOU 468	R CB HIS 5	7 4327 4959 432162 1000 36.99
ATOM 46	9 CG HIS 5	1 -11.004 -10.6 680 1344 -20.40
ANISOU 46	9 CG HIS 5	7 12 465 31 917 65 453 1 000 38 0 4
атом 47	0 NDI HIS	7 5090 4844 4823 -1/1 1362 137
ANISOU 47	O NEED TITO	67 - 10.70732.38764.2321.0011544 - 2828
ATOM 47	1 (1)	$\frac{419}{37}$ $\frac{434}{37}$ $\frac{1}{3000}$ $\frac{40.37}{37}$
ANISOU 47 ATOM 47	2 CE1 HIS S	1 - 11 - 12 1001 - 1001
ANISOU 47	2 CE1 HIS	57 5481 32 592 65.552 1.000 35.63
ATOM 47	3 NE2 HIS	D) =10+1
ANISOU 4	75 110 110	13 464 29 068 60 786 1 000 732 1 1525
ATOM 4	/ 4 1	58 4402 3186 4594 1 000 35 74
ANISOU 4		58 -14.290 20.732 4660 -1129 18// -1093
	75 CA GLY	58 4508 4402 11000 1 000 31 52
	76 C GLY	28 -73.443 -1.
ANISOU 4	76 C GLY	58 331, 245 26, 952 60, 922 1,000 32, 0 1012
$_{ m ATOM}$ 4	77 O GLY	58 4561 4176 3674 -204 624 13674
ANISOU 4	77 O GLY 78 N SER	59 -16.632 28.152 59.574 1.000 1142 -1442
ATOM 4 ANISOU 4		59 3786 3623 4379 50 859 1 000 32.03
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ANISOU	179 CA SER	59 3305 3323 = 2 417 1 000 37.27
MOTA	480 C SER	23 -1111 - 6607 11 2003 - 400-
ANISOU	480 C SER 481 O SER	59 -16.987 25.858 58.181 1.000 31.13 1003 -1174
ATOM	101	59 3027 3655 5104 1 000 39 80
ANISOU	481 O SER 482 CB SER	79 -17.01, -1
ATOM ANISOU	402 -	59 3930 5925 58 029 1.000 35.38
ATOM	483 OG SEK	
ANISOU	483 OG SER	59 3303 10 599 25 065 59.507 1.000 46.32
MOTA	484 N GLU	60 5438 6083 6078 -2395 2113
ANISOU	301	00 -10.3.3 - 4010 -960 /10
ATOM ANISOU	403	60 3381 4/98 40-000 1 000 34 22
ANISOU	486 C GLU	100 -10.000 10.00 10.00 0
ANISOU	486 C GLU	60 19 616 23.437 56.361 1.000 29.91
ATOM	487 0 616	1 60 3708 3040 4615 -679 2037
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ATOM 531 CB ALA 65 3096 2984 5993 1337 1401 ANISOU 531 CB ALA 65 3096 2984 5993 1337 1401 ANISOU 532 N VAL 66 -15.098 24.306 50.426 1.000 19.29 ATOM 532 N VAL 66 1836 1880 3614 466 360 -541 ANISOU 532 N VAL 66 1836 1880 3614 466 360 -541 ANISOU 533 CA VAL 66 -13.723 24.167 49.953 1.000 18.17 ATOM 533 CA VAL 66 1636 1653 3616 204 79 -487 ANISOU 533 CA VAL 66 1636 1653 3616 204 79 -487
ANISOU 531 CB ALA 65 3098 24.306 50.426 1.000 19.29 ATOM 532 N VAL 66 -15.098 24.306 50.426 1.000 19.29 ATOM 532 N VAL 66 1836 1880 3614 466 360 -541 ANISOU 532 N VAL 66 1836 1880 3614 49.953 1.000 18.17 ATOM 533 CA VAL 66 -13.723 24.167 49.953 1.000 18.17 ATOM 533 CA VAL 66 1636 1653 3616 204 79 -487 ANISOU 533 CA VAL 66 1636 1653 3616 204 79 -487
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ATOM 533 CA VAL 66 1636 1653 3616 204 75 18
NICOU 533 CA VAL 66 1636 1635 767 50.248 1.000 15.18
ATOM 534 C VAL 66 1516 1638 2613 120 120 63
ANISOU 534 C VAL 66 -11.959 22.623 50.353 1.000 17.100 -317
ATOM 333 0 WAL 66 1567 2071 3000 18 91
ANISOU 536 CB VAL 66 213 139 26 627 49.805 1.000 20.308 83
ATOM 537 CGI VAL 66 2067 1751 4010 219 321 61
NISON 538 CG2 VAL 66 2689 21 792 50.343 1.000 18.30
ATOM 539 N THR 67 1761 1614 3577 -20 17 18
ANISOU 539 N THR 67 13 673 20.403 50.563 1.000 17.556
ATOM 540 CA THR 67 1927 1656 294 332 1 000 16.52
CA1 C THR D/ -13.3.7.7 2000 21 2/ -40/
ANTSOU 541 C THR 67 1763 1742 48.811 1.000 18.13
ATOM 542 O THR 67 1750 2211 2929 73 86 3 54
ANISOU 542 OP THE 67 -14.373 19.791 51.702 193 224 -492
ATOM 543 CD TUP 67 2202 2014 2020 1 1 000 20 1 4
544 OC1 THR B/ TIE-000 T
ANISOU 544 OG1 THR 67 243 912 18 364 52.017 1.000 20.04
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5 A C N SER DO -13.000 - 130 134 22
ATOM 546 N SER 68 1612 1720 3010 16.33
ATOM 547 CA SER 60 1509 1631 3065 -184 30
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200M 549 O SER 08 14:303 1776 2659 -145 192
ATOM 549 O SER 68 1783 1775 2659 -143 172 ANISOU 549 O SER 68 1783 1775

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	\sim		- 31 - 17, 203	47 257	1.000 17.	84
ATOM 550	CB SER		958 17.303 2139			
ANISOU 550	CB SER	68 1459 68 -10.	998 18.259		1.000 17. -75 364	
ATOM 551 ANISOU 551	OG SER OG SER	co 1659	1987	2093	1 000 15.	89
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ANISOU 552	N PRO	69 1574 69 -15.	877 15.182	47.339	1.000 16. -251 -14	8 - 2 1 8
дтом 553	CA PRO CA PRO	60 1/128	1903	2900	1.000 17	. 2 2
ANISOU 553 ATOM 554	C PRO		.168 13.889 3 1578	2221	_199 200	
ANISOU 554	C PRO	69 1633 69 -15	794 12.99	7 48.287	1.000 18	. 3 5 - 3 7 6
ζζζ ΜΟπα	O PRO O PRO	60 181	5 1760	3333	-365 232 1.000 16	. 75
ANISOU 555 ATOM 556	CB PRO		.712 15.05 4 2279	2723	_36() 153) - 122
ANISOU 556	CB PRO		799 15.63	7 45.008	1.000 16 -359 38	. 12 - 452
дтОМ 557	CG PRO	60 155	3 1971	2021	1 000 17	. 1 0
ANISOU 557 ATOM 558	CD PRO	69 -15	.059 16.79 8 1804	2776	_ 3 4 4 - 1	<u> </u>
ANISOU 558	CD PRO	, <u> </u>	884 13.74	46 47.366	5 1.000 18 -89 29	2 -215
ATOM 555	N AVI	70 171	1764	3364	1 1.000 17	. 3 4
ANISOU 559	O CA VA	$\frac{1}{2}$ 70 $-\frac{1}{2}$	3.100 12.59 63 1851	~ ~ ~ 1	20 20	U +
ANISOU 56		^ 1	1.995 13.1		0 1.000 15 -180 15	17 + -
ATOM 56 ANISOU 56	<u>.</u>	70 22	იუ 1686	2100	9 1.000 1	3.59
атом 56	2 O VA		1.431 14.1 94 1688	2501	_ /1 (4) 1	J 4
ANISOU 56	2 O VA		2.429 11.7	57 46.72	4 1.000 1	30
ATOM 56 ANISOU 56	3 CB VA	L 70 19	22 1756 3.441 10.7		3 1.000 2	0.54
<u>атом</u> 56	54 CG1 VA	70 10	127 261.	3268	-369 7 12 1.000 1	0 - 0 0 2
ANISOU 56	64 CG1 VA 65 CG2 VA	70 -1	1.760 12.	608 45.64	7/5	1 0
ATOM 56 ANISOU 5	65 CG2 V	AL 70 2	379 180 11.697 12.	466 49.83	15 1.000 1	6.21 64 -156
атом 5	66 N P	no 71 1	653 181	0 2695	-34 4 -21 000 1	7.32
ANISOU 5 ATOM 5		RO 71 -	10.839 13.	~~~ 1	- 1 / 1	.04
ANISOU 5	67 CA P		795 193 9.356 12.	804 50.5	90 1.000	17.67
ATOM 5	68 C P	RO 71 1	865 192	27 2921	EO 1 000 3	20.5/
		RO 71 -			1 7 1	40 -
ANISOU 5	69 O E	PRO 71 2	11.362 12	.458 52.1	17 1.000	
ATOM ANISOU			180	62 2000	20 1 000	19.08
MOTA	571 CG	PRO 71	-11.721 11 2838 18	Λr 2603	8 -201	259 - 234 17.97
ANISOU	-	PRO 71 : PRO 71	-12.323 11	.220 50.	-390	451 -167
ATOM ANISOU	J / L	PRO 71	2314 19	74 253 .338 49.	446 1.000	17.15
MOTA	573 N		1677 22	31 261	0 -215	-17 -165 16.83
1,77,000	573 N 574 CA	THR 72 THR 72	-7.573 13	3.012 48.	0 -60	-134 - 4/2
ATOM ANISOU	574 CA	THR 72	1721 18 -6.490 14	000 49.	358 1.000	15.20 163 - 73
MOTA	575 C	THR 72 THR 72	1791 10	623 236	.104 1.000	17.49
ANISOU	575 C 576 O	THR 72	-5.320 1		<u> </u>	
ATOM ANISOU	576 0	THR 72	1776 1 -7.533 1	2.971 47	.399 1.000) 16.18 -86 -261
MOTA	577 CB	THR 72 THR 72	1552 1	848 27	.005 1.000	17.81
ANISOU ATOM	578 OG1	THR 72	-8.091 1	9gn 30	31 -34	110
ANISOU	578 OG	LTHR 72	-8.338 1	1.816 46	.825 1.00	0 17.49 181 -329
MOTA	579 CG	2 THR 72 2 THR 72	1953	2087 26	05 -550 9.987 1.00	0 17.78
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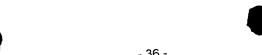




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ATOM 612 ANISOU 612	C GLY	76 1584 76 -7.469	2014 21.651	51.370 1.	000 16.87	- - ·
ATOM 613 ANISOU 613	O GLY	76 1638 77 -9.64	1998 3 22.025	51.863 1.	000 16.88 283 -191	•
ATOM 614 ANISOU 614	N PHE	77 1597	4 21.646	53.274 1.	00017.61	•
ATOM 615 ANISOU 615	CA PHE	77 1838	2196 6 20.154	53.512 1.	000 17.64	1 - 185
ATOM 616 ANISOU 616		77 1855	2248 389 19.528	52.831 1	000 18.2	3 - 2 4 0
ATOM 617 ANISOU 617	O PHE	77 1844	2488 598 22.383	53.998 1	.000 17.7	0
ATOM 618 ANISOU 618	CB PHI	E 77 1730	2515 877 22.081	1 55.473 1	.000 19.6	1 -516
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ATOM 62 ANISOU 62	O CD1 PH O CD1 PH	E 77 2514		2426 4 5 55.941 1	000 21.3	1
ATOM 62 ANISOU 62	1 CD2 PH	E 77 3282	2070 116 22.29	2743 4 57 742	1.000 21.	, •
ATOM 62 ANISOU 62	2 CE1 PH	IE 77 -10.	2768	1 57 300	171 221 1.000 25.	0 9
ATOM 62 ANISOU 62	3 CE2 PH	HE 77 296	7 4120 .175 21.52	2447	-501 625 1.000 23.	7 9
ATOM 62	24 CZ PI	HE 77 -11 HE 77 226	3 3681	3095	1.000 17	-
ATOM 63	25 N T	HR 78 -9. HR 78 161	6 2161	2925	1.000 18.	12
ATOM 6	26 CA T	HR 78 -9.	6 2243	2717	-157 624 1.00018	66
ATOM 6	27 C T	HR 78 -9	2308	2663	-367 519 1.000 21	. 4 2
	28 0	THR 78 -8	58 2883	3. 3098	1.000 21	.00
111000	529 CB '	THR 78 -8	73 206	7 2939	113 428	.18
MOTA	630 OG1 630 OG1	THR 78 -8	.027 17. 44 267	1 2833	0 1.000 26	. 65
MOTA	631 CG2	THR 78 -8	59 222	7 4141	-275 85	.36
ANISOU ATOM	632 N	GLY 79 -3	0.311 17. 569 23	2690	-6/0 03	96
ANISOU ATOM	633 CA	GLY 79 -	10.344 17 871 32	19 2745	-/90 37	7.0
ANISOU ATOM	634 C	GLY 79 -	10.029 16 407 35	42 5135	91 1.000 3	1.02
ANISOU ATOM	635 0	GLY 79 -		87 4272	36 1.000 3	6 07
ANISOU ATOM	636 N	LEU 80 -	380 45	36 4788	1381 -	2 52
ANISOU ATOM	637 CA	LEU 80	3640 40	83 4632	116 1 000 3	9.82
ANISOU ATOM	638 C	LEU 80	5051 4	652 5428	$\frac{1}{2}$	7.05
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ANISOM ATOM	640 CE	LEU 80	-7.122 1 3821 5	456 529	9 1568 883 1.000	
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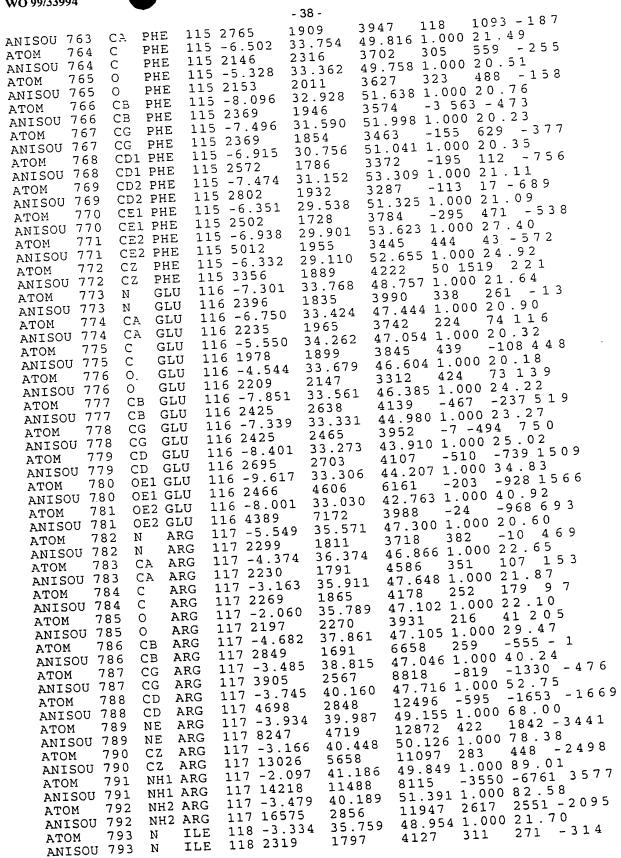


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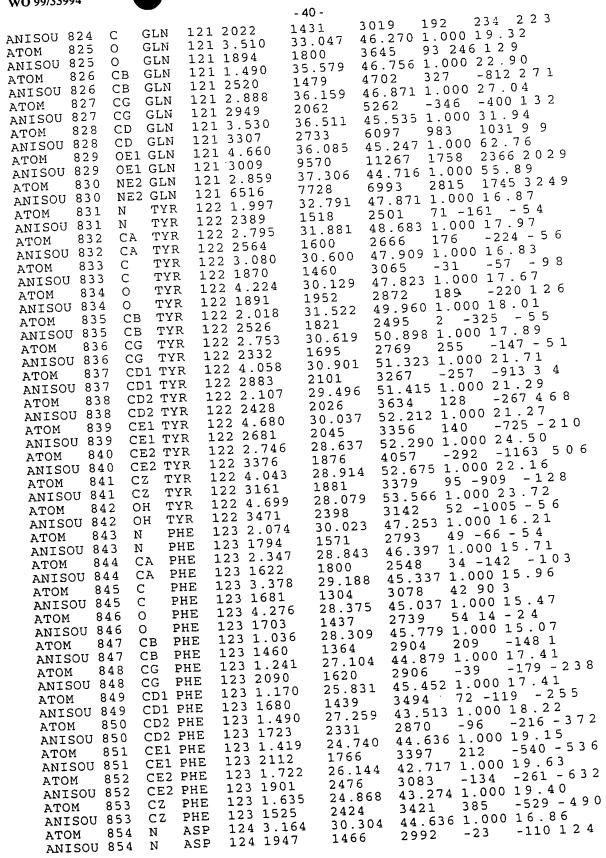


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ATOM 703 C ALA 106 1651	23 323 40.805 1.000 17.88
ATOM 704 0 ALA 106 2038	2087 2668 33 000 20 . 31
ANISOU 704 CB ALA 106 -4.862	2764 2620 -197 -403
ANISOU 705 CB ALA 106 2331	24.329 39.717 1.000 18.00
ATOM 706 N ASP 107 1576	2208 3037 1 000 17.46
ANISOU 707 CA ASP 107 -8.217	281 -83 -472 3 0 0
ANISOU 707 CA ASP 107 -8.173	23.753 41.859 1.000 1.269 3 6 2
ATOM 708 C ASP 107 1825	22 854 42.650 1.000 18.95
ATOM 709 0 ASP 107 1994	2230 2974 167 2133 2 2
ANISOU 709 U ASP 107 -8.089	
ANTSOU 710 CB ASP 107 2213	21 842 38.508 1.000 20.81
ATOM 711 CG ASP 107 1952	3093 2862 21300 25.84
ANISOU 711 OD1 ASP 107 -9.369	
ANISOU 712 OD1 ASP 107 -7.544	$\frac{21.168}{21.168}$ $\frac{37.844}{37.844}$ $\frac{1.000}{37.844}$ $\frac{23.00}{37.844}$
ATOM 713 OD2 ASP 107 3314	24 962 42 298 1.000 18 18
ATOM 714 N ASN 108 -7.89	2075 2786 509 17 10
ANISOU 714 N ASN 108 -7.83	1 23.203 2715 266 291 327
ANISOU 715 CA ASN 108 1804	9 25 716 44.314 1.000 17.11
ATOM 716 C ASN 100 1705	2061 2734 367 44 72
ANISOU 710 O ASN 108 -10.1	3430 759 22400
ANISOU 717 O ASN 108 2000	9 26.379 43.969 1.000 19.70
ATOM 710 CB ASN 108 1770	2308 333717 1.000 17.24
ATOM 719 CG ASN 108 -5.40	2212 2628 200 00 17 . 42
ANISOU 719 CO 118 108 -4.98	00 = - 6631 1119 11 0 -
ANISOU 720 OD1 ASN 108 2003	44 26 487 42.834 1.000 10.41
ATOM 721 ND2 ASN 108 2083	2326 2587 1 000 18.09
ATOM 722 N LEU 109 -9.3	2294 2786 349 344 11
ANISOU 722 N LEU 109 -10.	532 25.803 46.369 1.000 - 598
ANTSOU 723 CA LEU 109 176	169 26 790 47.457 1.000 17.40
ATOM 724 C LEU 109 1682	1937 2990 251 1000 21.18
ANISOU 724 C LEU 109 -9.	443 22
ANISOU 725 O LEU 109 244	100 24.504 46.940 1.000 17.10 630
ATOM /20 CB 227 100 188	8 2142 2409 1.000 18.07
ATOM 727 CG LEU 109 -11	5 1943 2409 1900 20 06
ANISOU 727 CG LEU 109 -11	
ANT COU 728 CD1 LEU 109 282	630 23 908 45 035 1 000 23 21 11
ATOM 723 035 100 341	81 2892 3211 1 000 17 25
ANISOU 729 CD2 PHE 110 -1	
ANISOU 730 N PHE 110 13	0.235 29.071 48.277 1.000 10.20
ATOM 731 CA PHE 110 17	51 1816 39 567 49.106 1.000 19.93
ATOM 732 C PHE 110 -1	11.407
ANISOU 732 C PHE 110 20	

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ATOM 733 O PHE 110 -12.433	2461 4851 612 328 - 773
ANISOU 7334 CB PHE 110 -9.607	3324 224 619 - 33
ANISOU 734 CB PHE 110 2367	29 986 46.688 1.000 19.47
ATOM 735 CG PHE 110 2009	2209 3179 -321 32/ -/91
ANISOU 735 CD1 PHE 110 -7.177	29.680 47.287 1.000 20.59 2080 3674 -274 236 -331
ANISOU 736 CD1 PHE 110 2071	30.035 45.299 1.000 20.19
ATOM 737 CD2 PHE 110 2557	1914 3200 112 343 -203
ANISOU 737 CE1 PHE 110 -6.034	3200 3673 -386 165 -622
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ATOM 739 CE2 PHE 110 2495	2138 3257 197 304 333
ATOM 740 CZ PHE 110 -6.081	3678 531 339 - 337
ANISOU 740 CZ PHE 110 2747	8 29.718 50.416 1.000 22.11
ATOM 752 21 DDO 111 2250	2153 3990 - 72 - 72 - 72 - 72 - 72 - 72 - 72 - 7
ATOM 742 CA PRO 111 -12.28	2210 4621 698 1514 - 671
ANISOU 742 CA PRO 111 3833	3 31.866 50.784 1.000 30.57
A10M / 10 0 DBO 111 4528	2026 5001 415
ATOM 744 O PRO 111 -11:33	$\frac{1}{2}$
ANISOU 744 CB PRO 111 -11.79	9 30.250 52.627 1.000 33.20
ANISOU 745 CB PRO 111 5609	2702 4303 0.1 000 26.04
ATOM 746 CG PRO 111 -10.0	3316 3835 -931 1324 -192
ANISOU 740 CD PRO 111 -10.16	
ANISOU 747 CD PRO 111 2587	37 32.641 51.150 1.000 42.13
ATOM 110 N CEP 112 7176	2/16 50 672 1 000 44 . 05
ATOM 749 CA SER 112 -13.3	7684 1107 -485 -820
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ANISOU 750 C SER 112 13632	4498. 7812 1000 95.18
ATOM 751 O SER 112 12.3	11425 8747 -4337 -70 1983
ANISOU 751 CB SER 112 -12.4	193 35.069 51.349 1.000 1662 -1437
ANISOU 752 CB SER 112 224/	174 34 624 52.213 1.000 37.49
ATOM 753 OC SER 112 7213	2453 4579 806 747 -1132
ATOM 754 N ASP 114 -9.5	6446 9747 1734 403
ANISOU 754 N ASP 114 3476	05 37.586 50.600 1.000 30.79
ATOM 755 CA ASP 114 3503	2856 5340 1220 26.16
ATOM 756 C ASP 114 -7.2	4955 601 1114 8 0 4
ANISO0 757 O ASP 114 -6.0	31 36.458 50.338 1.000 25.43
ANISOU 757 O ASP 114 2302	2503 4800 1.000 43.68
ATOM 758 CB ASP 114 750	2783 6304 1157 2727 2210
ANISOU 750 CG ASP 114 -7.3	$391 \ 38.386 \ 52.833 \ 2517 \ 519 \ 107$
ANISOU 759 CG ASP 114 925	38.959 52.189 1.000 83.49 30.56
ATOM 760 OD1 ASP 114 137	24 9866 8132 -6354 636
ATOM 761 OD2 ASP 114 -7.	10550 4730 -6984 -109 -23
ANISON 761 DE PHE 115 -7.	831 35.323 51.153 1.000 22.32
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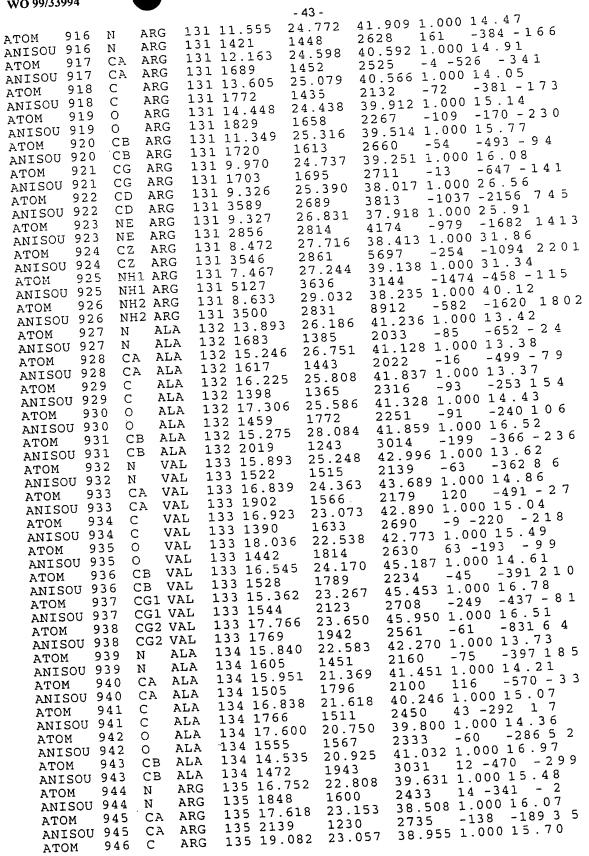


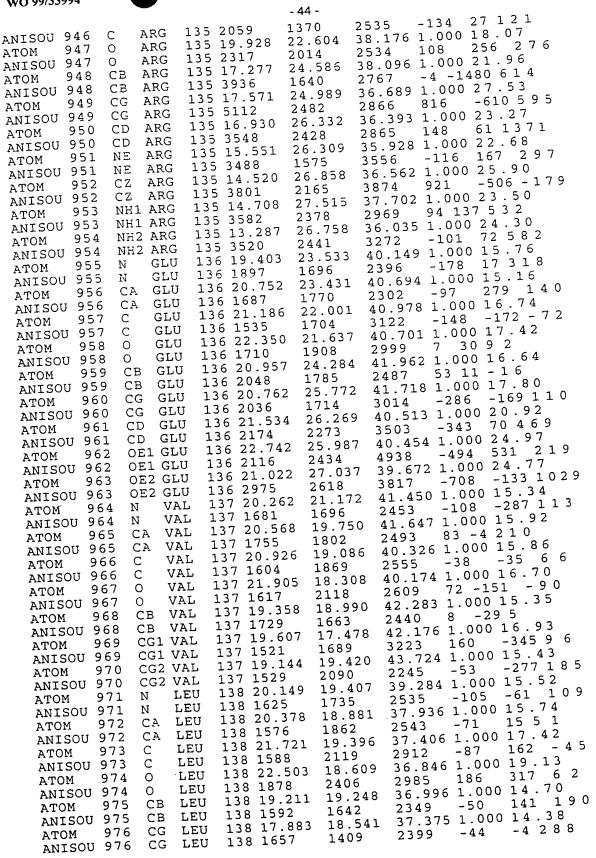
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ATOM 8 ANISOU 8 ATOM 8 ANISOU 8 ATOM 8 ATOM 8	116 CA 1 116 CA 1 117 C 1 117 C 1 1318 O 1 1818 O 1 1819 CB 1	HR 120 1915 HR 120 -0.5 HR 120 203 HR 120 0.7 HR 120 199 HR 120 -2. THR 120 195	5 2469 169 32.5 1 1855 00 31.9 6 1887 487 32.8	2398 87 45.288 2629 60 44.674 7 3212 365 44.344 2720	1.000 17.15 241 -155 1 9 2 1.000 18.67 389 -131 1 7 7 1.000 18.10 28 -93 3 4 5
ATOM ANISOU ATOM ANISOU ATOM ANISOU ANISOU ATOM ANISOU ATOM ANISOU	820 OG1 820 OG1 821 CG2 821 CG2 822 N 822 N 823 CA 823 CA	THR 120 180 THR 120 -1	7 280 .919 32. 38 326 .94 33. 80 165 466 34. 77 169	1 3179 803 42.933 6 2830 708 45.95 7 3237 232 45.99	59 -363 558 31.000 22.46 475 118 705 61.000 18.62 123 -94 213 31.000 18.15 77 96 5 20 81.000 17.04
ATOM	824 C				



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- 41 -
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                    124 4.060
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           CA ASP
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MOTA
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                                2636
            OD1 AASP 124 2189
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ANISOU 860
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MOTA
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CB BASP 124 2559
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ATOM
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CG BASP 124 3552
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 MOTA
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OD2 BASP 124 3845
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                 ARG
                                                      91 - 233
        869 0
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 MOTA
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                                 32.468 46.851 1.000 20.45
                      125 1639
                 ARG
 ANISOU 869 O
                      125 7.062
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        870 CB ARG
870 CB ARG
 MOTA
                                  2162
                      125 2219
                                 33.916 46.344 1.000 28.23
 ANISOU 870 CB
                      125 6.860
                                                      666 - 222
             CG
                ARG
         871
                                                147
 MOTA
                                          5542
                      125 3178
                                  2007
                                  34.891 47.477 1.000 31.76
                ARG
 ANISOU 871
             CG
                      125 6.693
                                                      1455 - 993
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                                                -628
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             CD
 MOTA
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                                  36.221 46.932 1.000 40.81
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         873
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             ΝE
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             CZ
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                                                       1627 - 681
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                        126 5.208
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                                    2670
                        126 2957
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ATOM 886 N TYR 127 1629	1436 2430 1 000 13.93
ANISOU 887 CA TYR 127 7.039	
ATOM 007 C3 TYR 127 1563	1400 227,
ANISOU CO C TYR 127 8.289	$\frac{1}{2}$
TYR 127 1461	1318 2745 24 -193 1 3 9 26.345 42.140 1.000 14.39
	34 - 252 9
ANTSOU 889 O TYR 127 1611	56 676 42 435 1,000 14.00
ATOM 890 CB TIR 127 3:00-	2258 29 -180 - 70
ANISOU 890 CB TYR 127 1313	25.795 41.202 1.000 12.33
ATOM 891 CG TYR 127 3.752	1037 2334 -34 -107 = 3
ANISOU 051 1 TVD 127 6 483	24.626 41.024 1.000 14.03
ATOM 852 CD 127 1910	1158 2371 / -84 - 3
ANISOU 032 CD2 77 1 27 4 837	7 26.086 40.206 1.000 15.71 1548 2484 55 -513 2 1
A.LOM 833 624 - 102 1036	1548 2464 33 22 10
ANISOU 093 CE1 TYR 127 6.382	2 23.829 39.899 1.000 13.10 999 2529 -101 -227 -62
ATOM 604 CE1 TYR 127 1450	999 2529 -101
ANISOU 894 CE2 TYR 127 4.66	
ATOM 205 CE2 TVR 127 1928	1620 22 034 1 000 13.71
AN1000 006 C7 TYR 127 5.44	2245 -146 -100 2 4 0
ANTSOU 896 CZ TYR 127 1617	27 811 1 000 15.04
ATOM 897 OH TYR 127 3:33	7 7955 2279 -87 -60 3 3
ANISOU 897 OH TYR 127 1002	28.412 42.616 1.000 14.03
ATUM 000 1012	1324 2446 -154 -217 67
ANISOU 000 AN MUD 128 9 67	73 28.984 42.011 1.00 32 1.95
ATUM 800 CA THR 128 1867	1 1469 2236 1 000 14 68
ANISOU 000 C THR 128 10.9	$\frac{921}{28.552}$ $\frac{42.750}{2466}$ $\frac{1.5}{59}$ $\frac{1}{23}$ $\frac{1}{285}$
ATOM 000 C THR 128 179	4 1310 - 200 1 000 15 45
ATOM 901 0 THR 128 11.	2667 -259 133 / 1
ANTSOU 901 O THE 120 1/1	72 30 544 42.069 1.000 16.02
ATOM 902 CB THR 120 314	72
ANISOU 302 021 MUD: 128 8 5	19 30.849 41.162 1.000 13.14
ATOM 903 OC1 THR 128 222	6 2038 - 3000 19.03
ANISOU 903 CG2 THR 128 10.	835 31.18/ 41.382 1.38 311 618
ATOM 904 CC2 THR 128 210	1329 3793 12000 14.21
205 N ALA 129 10.	2424 -137 -250 -101
AT.A 129 1/0	100 20 110 44.836 1.000 15.08
ATOM 906 CA ALA 129 12	-118 -210 -225
ANISOU 906 CA ALA 129 10	399 26.643 44.562 1.000 14.37
ATOM 907 C 122	06 1299 2457 -159 -203 1 3 7
ANISOU 307 0 ATA 129 13	.552 26.238 44.443 16 244 -148
ATOM 900 0 ATA 129 17	$\frac{1464}{6}$ $\frac{213}{6}$ $\frac{1}{213}$ $\frac{1}{1}$ $\frac{1}$ $\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$
ANISOU 500 CB ATA 129 11	.887 28.313 46.313 1.83 -514 - 239
A10M 000 CB ALA 129 21	32 1031 44 553 1 000 14 . 18
ATOM 910 N SER 130 11	$\frac{1.343}{20.01}$ $\frac{23.01}{2267}$ $\frac{-224}{-257}$ $\frac{-257}{1}$
ANTSOU 910 N SER 130 18	375 44 351 1.000 15 44
ATOM 911 CA SER 130 13	2007 -115 -135 - /
ANISOU 911 CA SER 130 13	2.072 24.114 42.965 1.000 14.43
ATOM 912 C C 120 1	345 1481 2665 76 27 30
ANISOU 912 C SER 130 1	3.037 23.329 42.807 1.000 -246 1.72
ATOM 513 0 SFR 130 1	$\frac{1382}{1382}$
ANISOU 913 CB SER 130 1	0.120 23.6// 44.003 1.79 -647 1 2 6
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ATOM 915 OG SER 130 2	
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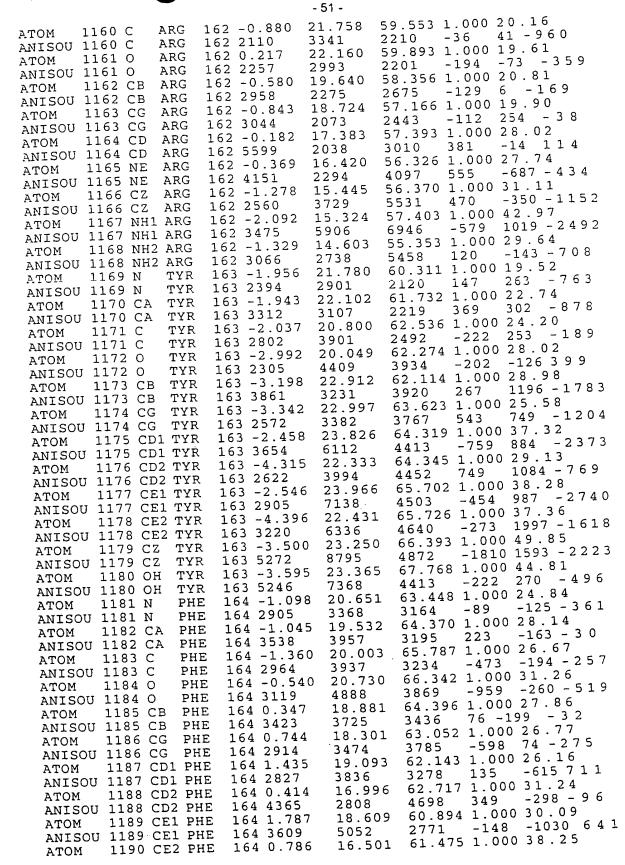




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ATOM 978 CD2 LEU 138 17.9	1425 3021 -107 -486 207
ANISOU 978 CD2 LEU 138 2185	62 20 708 37 548 1.000 17.44
ATOM 979 N ARG 139 21.3	$\frac{2}{2}$
ANISOU 979 N ARG 139 1797	89 21 319 36.996 1.000 19.00
ATOM 980 CA ARG 139 23.1	$\frac{2}{3}$ $\frac{2}$
ANISOU 300 CI. 130 24 4	19 20.734 37.685 1.000 19.72
ATOM JOE C	2600 3097 -518 482 3 7 6
ANI300 301 3 220 25 4	61 20.432 37.094 1.000 207.10
ATOM 982 O ARG 139 2046	2469 3350 -288 607 23
AN1300 983 CB ARG 139 23.1	102 - 102 402 951 691
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ATOM 984 CG ARG 139 23.0	2007 4212 -2176 1609 1 4 0
ANISOU 984 CG ARG 139 651	25 140 26 443 1 000 44 . 95
ATOM 985 CD ARG 139 23.0	7716 -242 -1324 1930
ANISOU 985 CD ARG 139 745	525 25.727 36.547 1.000 43.27 CDB
ATOM 300 III	5959 -828 -21/3 - 939
ANISOU 700 12 120 21	821 26.330 35.605 1.000 41.34
ATOM Jon	9 4102 5666 497 310 4101
ANISOU 988 NH1 ARG 139 22.	308 26.436 34.376 1.000 1393 3 3 6
ATOM 900 NH1 ARG 139 656	4 4146 6011 330 45.75
ATOM 989 NH2 ARG 139 20.	537 1938 2403
ANISOU 989 NH2 ARG 139 616	2 4616 30 009 1 000 18.77
ATOM 990 N ALA 140 24.	2207 3003 -255 145 0 3
ANISOU 990 N ALA 140 1/4	532 20 169 39.773 1.000 19.53
AIUM JJE GEO	3197 -28 38 - 666
ANISOU 331 CH NEN 140 25	932 18.732 39.490 1.000 18.30
ATOM 992 C ALA 140 201	L8 2342 2843 -67 78 -103
ANISON 993 O ALA 140 27	109 18.335 39.626 1.000 21.00
ALA 140 190	2430
ATOM 994 CB ALA 140 23	3084 35 0 - 360
ANISOU 994 CB ALA 140 18.	250 17 943 39.062 1.000 20.32
ATOM 995 N THR 141 24	2000 3498 -115 305 -130
AN 1300 333 A BYED 141 25	151 16.530 38.717 1.000 17.15
AIOM 330 CT	70 2039 2609 61 51 21 6
ANISOU 330 CI MUD 141 25	.269 16.278 37.208 1.000 1.000
ATOM 997 C THR 141 14	92 2443 2693 21 270 19 24
ANISON 998 O THR 141 25	
ANTSOU 998 O THR 141 18	3/1 2023 39 290 1.000 16.79
ATOM 999 CB THR 141 24	2410 83 164 3 1
ANISOU 999 CB THR 141 17	788 16.012 38.710 1.000 17.18
ATOM 1000 CC - 1	2399 -101 -53 5 + 6
ANISOU IOOO OOL III	3.982 15.734 40.807 1.000 17.83 2.000 2.000 17.83 2.000
ATOM 1001 CG2 THR 141 1	$\frac{2878}{2377}$
AN1300 1002 N GLY 142 2	5.361 17.301 36.381 1.000 302 297
NITCOU 1002 N GLY 142 2	091 2789 2603 1,000 19.08
ATOM 1003 CA GLY 142 2	2551 128 -103 4 3 3
ANISOU 1003 CA GLY 142 1	8/8 2819 2332 1.000 18.75
ATOM 1004 C GLY 142 2	2744 0 252 -11/
ANISOU 1001 C	14 443 15.755 33.315 1.000 22.41 cso
AIOM 1000	2432 2681 3403 -161 5/1 -000
AN 1300 1000 0 mrp 1/3 2	23.093 16.650 34.854 1.000 17.20
ATOM 1006 N THR 143 1	L895 2002 2667 67 300 2 1 2
ATOM 1007 CA THR 143	21.909 15.932 34.393 1.000 16.80
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ANTSON 1007 CA THR 143 1953	2006 2456 104 17 03
ANISOU 1007 C.1	16.660 33.432 1.000 17.02
A 17 () (4)	1/22 30
ANISOU 1000 0 my 143 20 457	17.713 33.764 1.000 20.30 17.713 31.764 12 - 28
A-1-()M 1000 0	1013 3103 100 10 40
ANISOU 1000 - WYD 143 21 085	15.490 35.623 1.000 16.40
A.T.O.M. 1010 02	2329 2130 - 222 17 22
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ATOM 1011 OG1 THR 143 2009	20/3 2000
ANISOU 1012 CG2 THR 143 19.887	
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- mon 1013 N GLU 144 20.742	
-XTCOU 1013 N GLU 144 2138	2200
2 mom 1014 C2 GLU 144 19.729	$\frac{1}{2}$
1014 CA GLU 144 2202	15 506 31 354 1 000 19.18
ATOM 1015 C GLO 144 10.03	-2.614 -2.418 -2.92 -2.30 -1.31
ANISOU 1015 C GLU 144 2233	14 420 30 665 1 000 21 46
ATOM 1016 O GLU 144 10.02	5445 3446 19 649 - 88
ANTSOU 1016 0 GLU 144 2200	17 061 30.006 0.753 29.50
ATOM 1017 CB AGLU 144 20.230	1266 -855 206 I 3 0 I
AN 1500 101 100 101 100 105	
	3913 3913 -1728 1769 793
ANTEGO 2010 CD 3CT II 144 21 242	19.411 30.426 0.753 33.13
	3432 4966 104 744 001
ANISOU 1000 001 2011 144 21 079	9 19.690 31.641 0.753 51.91 11101 4940 -868 -202 -590
ATOM 1020 OF LAGIN 144 3684	11101 4940 -005 50 79
1021 OF2AGLU 144 44.40	
1021 OF2AGLII 144 /949	2022
1000 CD B(-1.0 144 40.0)	3016 334 16264
DOTT 1// SEX 1	
ATOM 1023 CG BGLU 144 21.21	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ANTSOU 1023 CG BGLU 144 1301	0 18 468 28.336 0.247 33.24
ATOM 1024 CD BGLU 144 21-15	2025 5064 438 -20 2031
ATOM 1024 CD BGLU 144 3589 ANISOU 1024 CD BGLU 144 20.41	7 17.818 27.557 0.247 28.68
	4813 2861 389 1725 25
ANISOU 1023 0220 144 21 81	4 19.464 27.990 0.247 33.33
AION 1020 0 144 2176	5148 5108 33 17 11
ANISOU 1020 DDO 145 17 50	1825 2543 68 62 1 5 8
ATOM 1027 N PRO 145 2132	1825 2543 00 02 17 41
2 mov 1028 CA PRO 143 10.3	73 400 1 4
	1942 2304 1 000 17.94
ATOM 1029 C PRO 145 15.9	2475 -116 494 -+ 4
ANISOU 1029 C PRO 145 2386	68 15 439 29.557 1.000 18.26
ATOM 1030 O PRO 145 10.0	2472 -272 1/0 4 3
ANISOU 1030 O PRO 145 22/1	55 402 32 594 1 000 17 . 07
AIUM 1031 02 - 145 0101	75 1991 2534 35 133 - 143
ANISOU 1031 CD 145 15 0	50 16.504 33.464 1.000 17.11
A LUM 1000 00 1 1 2 2 2 4	
ANISOU 1032 CD DDO 145 17	131 16.977 32.649 1.000 17.33 3 3 3
ATOM TOJS CD	3 1601 2884 176
ANISOU 1033 N ASP 146 15.	490 13.346 30.104 1.000 321 -152
ATOM 1034 N ASP 146 214	0 1965 2790 200 18.43
AN1300 1031 CA ASP 146 14.	909 13.121 28.775 1.000 310 -156
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ATOM 1036 C ASP 146 13.	2064 -31 208 -309
ANISOU 1036 C ASP 146 282	19/9 2004 1.000 18.29
ATOM 1037 O ASP 146 12.	168 703 -430
ANISOU 1037 O ASP 146 249	1

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ANTSOU 1129 CA BEO 133	1333 2033 1.000 14.49
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ANISOU 1130 C BEU 159 -0.790	21.596 49.419 1.000 13.09 0
ATOM 1131 O LEU 159 1414	1999 2319 20 1 29
ATOM 1132 CB LEU 159 1.390	1447 2639 55 -325 - + 7 /
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ATOM 1133 CG LEU 139 1.404	1600 2665 363 -332 -343
ANISOU 1133 CG 1120 159 2.775	24.114 50.453 1.000 18.70
ANTSOU 1134 CD1 LEU 159 2276	25 201 49 291 1 000 21.00
ATOM 1135 CD2 LEU 139 1.312	1525 3526 439 -692 - 3 6 2
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A1011 1130 1	1709 2063 -101 -100 4 /
ANISOU 1137 CA ARG 160 0.055	20.747 51.901 1.000 15.61 1990 2217 -64 90 -118
ANISOU 1137 CA ARG 160 1/26	1990 2217
ATOM 1138 C ARG 100 0.400	-34 - 45 - 30
ANISOU 1130 0 ARC 160 1 639	21.401 53.576 1.000 16.32
ATOM 1139 O ARG 160 1528	2508 2164 63 41 - 104
200M 1140 CB ARG 100 0.040	$\frac{1012}{1012} - \frac{127}{12} - \frac{30}{12} = \frac{12}{12}$
ANISOU 1140 CB ARG 160 2134	18 410 51.155 1.000 17.17
A1()(1) 1111 ()	1934 2628 -140 -212 -60
ANISOU 1141 CD ARG 160 -0.672	16.959 51.627 1.000 18.16 18.955 2166 125 -330 - 3.5
ANISOU 1142 CD ARG 160 2767	16 102 50 682 1.000 18.11
ATOM 1143 NE ARG 160 -1.382	1885 2600 -56 -308 4 V
ANISOU 1113 17 170 160 -1 221	14.789 50.581 1.000 16.76
ATOM 1114 CZ ARG 160 2191	1748 2428 1374 1 000 20.55
ATOM 1145 NH1 ARG 100 -0.320	-26 -45/303
ANISOU 1145 NH1 ARG 160 2300	14.095 49.689 1.000 19.23
ATOM 1146 NH2 ARG 160 -1.908 ANISOU 1146 NH2 ARG 160 2502	2031 2774 181 -147 - 336
AMISOU 1147 N PHE 161 -0.469	7111 -37 -63 -120
ANISOU 1147 N PHE 161 1604	2120 2111 000 16.25
ATOM 1148 CA PHE 161 -0.20.	2227 -71 -18/ - 83
ANISOU 1110 C. DUR 161 -1 031	0 22.236 56.069 1.000 16.36
ATOM 11/49 C PHE 161 1980	2432 2041 -217
ATOM 1150 O PHE 161 -2.24	$\frac{1}{2}$
ANISOU 1150 0 PHE 161 1901	3 24.431 54.862 1.000 19.70
ATOM 1151 CB PHE 161 2065	1903 3540 167 333 61
ATOM 1152 CG PHE 161 -0.37	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
ANTSOU 1152 CG PHE 161 3026	25 304 57.228 1.000 28.25
ATOM 1153 CDI PHE 101 -1-1-	1269 1077 369 -1233
ANISOU 1153 CD1 PHE 161 3992 ATOM 1154 CD2 PHE 161 0.807	7 25.978 56.141 1.000 26.02 927 = 1.06
ANTSOU 1154 CD2 PHE 161 4015	2483 3616 -130 35 29
ATOM 1155 CEL PHE 101 -0.0.	1538 -135 -135
AN1300 1135 CD2 DUE 161 1 15	3 26.723 57.258 1.000 33.63
ATOM 1156 CE2 PHE 161 4643	3240 4894 1205 200 44
ATOM 1157 CZ PHE 101 0.32	1000 3403 1455 -24//
ANISOU 1157 CZ PHE 161 60/1	58 21.767 57.130 1.000 17.59
ATOM 1158 N ARG 162 -0.5	2487 2103 -118 -135 - 6 9
ANTISOU 1159 CA ARG 162 -1.0	072 21.078 58.199 1.000 18.27
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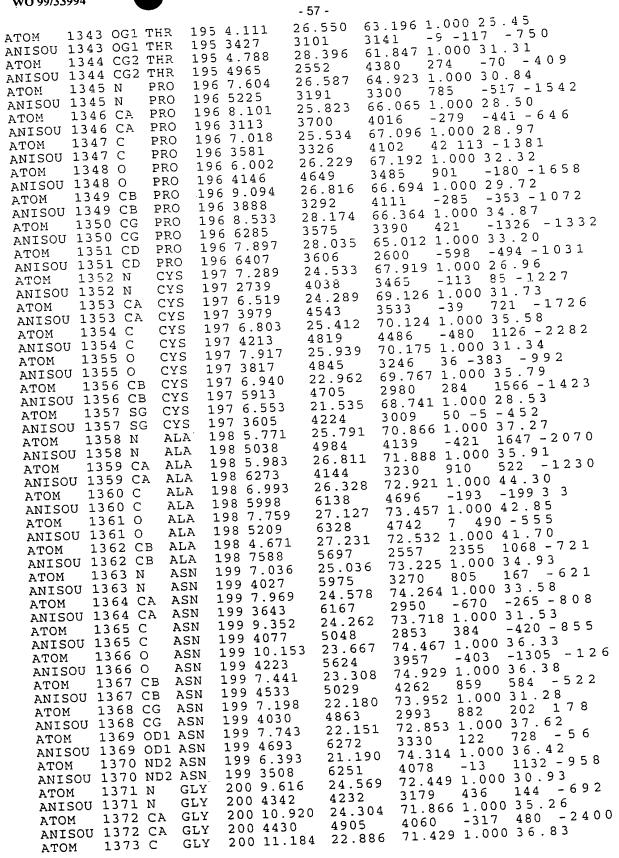
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1101 C7 PHE 164 3187	50/8 41/2 1.000 30.62
N PRU 103 - 2:103	1000 2751 -1371 344 - 500
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ATOM 1193 CA PRO 165 22.070	7510 -190 80 2 3 9
ANTSOU 1193 CA PRO 103 3233	19 408 68.638 1.000 36.32
27()[1] 2232	
ANISOU 1134 C 776	18.428 68.371 1.000 32.94
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ANISOU 1196 CB PRO 165 -3.882	765 373 877
ATOM 1196 CB PRO 165 3807	6924 3873
ATOM 1197 CG PRO 103 -4.033	7020 3995 5 688 - 8 2 8
ANTSOU 1197 CG PRO 103 2373	10 130 65 710 1.000 33.90
ATOM 1198 CD PRO 103 -3.000	5010 3770 -1149 194 1 6 9
ANISOU 1100 UL 178 7 727	7.453 68.180 1.000 64.52
A 1 () M	5376 6843 278 -216 3721
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ATOM 1200 CA LEU 178 10557	2/30 3100
1201 C LEU 1/8 6.159	2520 5225 -2598 -1186 1204
ANISOU 1201 C LEU 178 9239	55 796 1 000 56.53
ATOM 1202 O LEU 1/8 3.314	7076 -4835 1265 - 602
ANISOU 1202 0 TEIL 178 8 222	7.582 65.746 1.000 55.55
AT()M 1203 C2	3734 5902 -1314 -1137
ANISOU 1203 CG LEU 178 9.662	7.092 65.774 1.000 62.34 5116 7760 -1971 194 -443
ATOM 1204 CG LEU 178 10812	54 579 1 000 54 . 23
ATOM 1205 CD1 LEU 1/8 9.310	1000 1000 1878 -3/99 511
ANTSON 1205 CD1 LEU 1/8 9020	4905
ATOM 1206 CD2 LEU 178 10.05	10526 -1170 4090 -310
ANISOO 1200 022 ARC 179 5 879	9.751 66.192 1.000 52.30 10.31
ATOM 1207 N ARG 179 7853	3826 8421 102 120
ANISOU 120, CA ARG 179 4.495	10.000 7421 -229 1890 -383
ANISOU 1208 CA ARG 179 7235	0 563 64 383 1.000 55.25
ATOM 1209 C ARG 1/9 4.242	7731 -946 2260 -1134
ATOM 1209 C ARG 179 7178 ANISOU 1209 C ARG 179 3.120	9.211 64.021 1.000 58.51
AIUM 12100	7628 7565 -1820 3073 200
ANISOU 1210 CB ARG 179 4.180	11.512 66.040 1.000 41.49 4448 4716 -155 1916 1137
ATOM 1211 CB ARG 179 6600	4448 4/16 2133 1323
200M 1212 CG ARG 1/3 3.42	7 = 000 4367 90 1338 9 3 0
ANISOU 1212 CG ARG 179 6120	350 66 833 1 000 47 .63
ATOM 1213 CD ARG 1/9 1.800	7 7 4463 195 860 -334
ANISOU 1213 01 170 1 45	9 13.367 67.269 1.000 52.00 53.8
ATOM 1214 NE ARG 179 7384	7834 4539 1000 2-1
ANISOU 1211 CZ ARG 179 1.32	2 14.470 66.556 1.667 -1107 6 3
ANTSOU 1215 CZ ARG 179 1083	8 8000 - 57 360 1 000 59 74
ATOM 1216 NH1 ARG 1/9 1.03	3628 -4031 4 4 3
ANISOU 1216 NH1 ARG 179 9533	15.606 67.117 1.000 65.83
	51 9083 5478 4171 -776 1200
ANISOU 1218 N MET 180 5.30	04 9.501 63.509 1.500 852 -1245
ATOM 1218 N MET 180 538	3 3769 7550 705 350
ATOM 1219 CA MET 180 3.2	75/3 -398 5/4 -1402
ANISOU 1219 CA MET 180 235	61 920 1,000 43.91
ATOM 1220 C MET 180 6.5	26 - 1 19 370 - 2324
ANISOU 1220 C MET 180 2/3	

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22.7.1.000.39.46
ATON 1221 O MET 180 7.629 8.679 62.327 1.000 39 .46 ANTON 1221 O MET 180 2377 5064 7554 93 506 -912 ANTON 1222 CB MET 180 5.129 10.189 61.219 1.000 49 .84 ATON 1222 CB MET 180 7.249 7966 8223 7.71 0.00 62 .58 ATON 1223 CG MET 180 7.280 911 7966 822 7.71 0.00 62 .58 ANTON 1223 CG MET 180 7.280 911 758 68 823 7.77 1.000 62 .58 ANTON 1224 SD MET 180 4.622 11.015 758 68 823 7.77 1.000 62 .58 ANTON 1224 SD MET 180 4.622 11.015 758 68 1.000 74 .24 ANTON 1225 CE MET 180 4.621 11.015 758 68 1.000 74 .24 ANTON 1225 CE MET 180 4.501 1.000 77 1.000 62 .58 ANTON 1226 N ALA 181 6.376 7.112 1.000 79 .59 ANTON 1227 CA ALA 181 7.407 980 980 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.407 980 505 5 -271 882 -1112 ANTSOU 1227 CA ALA 181 7.407 980 505 5 -271 882 -1112 ANTSOU 1227 CA ALA 181 7.407 980 505 5 -271 882 -1112 ANTSOU 1227 CA ALA 181 7.804 650 1 800 7.000 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.804 7.305 6.100 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.804 7.305 6.100 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.804 7.305 6.100 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.804 7.305 6.100 6250 -625 2048 46 1 ANTSOU 1227 CA ALA 181 7.804 7.305 6.100 6250 -625 2048 46 1 ANTSOU 1228 C ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 6.727 4.817 7.305 6.500 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 1.305 7.305 6.200 6250 -625 2048 46 1 ANTSOU 1230 CB ALA 181 1.305 7.305 6.200 6.200 0.000 42.66 6 ANTSOU 1230 CB ALA 181 1.305 7.305 6.200 6.200 0.000 42.66 6 ANTSOU 1230 CB ALA 181 1.305 7.305 6.200 0.000 42.66 6 ANTSOU 1230 CB ALA 181 1.305 7.305 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.600 6.200 0.000 22.6
ATOM 1251 O TIR TOT STORY

- 54 --103 -448 150 2916 1383 184 1717 TYR 51.360 1.000 15.66 ANISOU 1251 O 184 12.699 8.004 TYR 1252 CB 69 -366 -168 2943 184 1686 1323 TYR ANISOU 1252 CB 50.562 1.000 14.85 6.785 184 12.383 1253 CG TYR -567 4 MOTA 109 1313 2586 184 1743 ANISOU 1253 CG 51.185 1.000 15.49 TYR 184 12.200 5.540 -29 -575 1 9 0 1254 CD1 TYR MOTA 3021 1315 184 1549 ANISOU 1254 CD1 TYR 49.165 1.000 15.89 184 12.329 6.836 1255 CD2 TYR 55 -27 - 64 ATOM 2552 1763 184 1724 ANISOU 1255 CD2 TYR 184 11.962 4.396 50.442 1.000 15.61 1256 CE1 TYR -137 1 1 3 MOTA 2992 229 1244 184 1695 ANISOU 1256 CE1 TYR 48.447 1.000 17.52 184 12.130 5.661 1257 CE2 TYR 4 83 - 90 2540 184 2340 1776 ANISOU 1257 CE2 TYR 49.083 1.000 16.96 184 11.915 4.449 TYR-156 -480 3 4 1258 CZ MOTA 3014 1736 184 1695 TYR ANISOU 1258 CZ 184 11.682 3.325 48.310 1.000 18.81 1259 OH TYR -277 - 312 3352 260 ATOM 1775 184 2020 185 10.924 10.330 50.502 1.000 14.36 ANISOU 1259 OH TYRASP 87 - 225 276 1260 N MOTA 2338 1599 185 1518 ASP 185 10.026 11.005 49.574 1.000 13.88 ANISOU 1260 N 1261 CA ASP -364 - 42 MOTA 141 2078 185 1875 1322 ANISOU 1261 CA ASP 185 10.240 10.490 48.152 1.000 12.57 -160 -77 -130 ASP MOTA 1262 C 1385 2211 185 1182 185 11.357 10.135 47.824 1.000 14.14 ANISOU 1262 C ASP ASP -135 146 140 1263 0 MOTA 2559 1637 185 1177 49.580 1.000 14.97 ANISOU 1263 O ASP 185 10.294 12.521 ASP -186 - 159 1264 CB MOTA 121 2517 185 1879 1293 13.155 50.830 1.000 17.61 ANISOU 1264 CB ASP 185 9.702 -13 -172 1265 CG ASP 232 MOTA 2351 1659 185 2680 ANISOU 1265 CG ASP 12.466 51.856 1.000 23.69 185 9.507 1266 OD1 ASP -302 5 2 1 MOTA 443 2314 3133 185 3553 14.257 50.742 1.000 24.32 ANISOU 1266 OD1 ASP 185 9.174 1267 OD2 ASP 1140 - 16 644 MOTA 1730 3449 185 4063 186 9.141 10.465 47.382 1.000 12.57 ANISOU 1267 OD2 ASP -117 -117 -117 LEU 1268 N MOTA 2126 1378 186 1271 10.091 45.986 1.000 12.92 ANISOU 1268 N LEU 186 9.169 -331 -84 -175 LEU 1269 CA ATOM 2150 1225 186 1533 11.292 45.052 1.000 14.12 ANISOU 1269 CA LEU 186 9.134 -165 5 5 LEU 1270 C MOTA -93 1307 2330 186 1730 1307 2330 -93 186 8.971 11.173 43.849 1.000 20.12 2280 -423 99 9 2 LEU ANISOU 1270 C LEU 99 9 2 1271 0 ATOM 2280 1643 186 3721 45.609 1.000 13.72 ANISOU 1271 O LEU 9.106 186 8.040 LEU -375 -1272 CB -270 MOTA 2393 1310 186 1509 46.438 1.000 15.92 ANISOU 1272 CB LEU 7.811 186 8.020 1273 CG LEU -145 -307 1 6 8 MOTA 3361 1141 186 1549 LEU 45.866 1.000 19.36 ANISOU 1273 CG 6.908 186 6.929 3825 -700 -209 3 9 6 1274 CD1 LEU MOTA 186 1686 1845 ANISOU 1274 CD1 LEU 46.341 1.000 18.32 7.115 186 9.369 200 -432 1 7 9 1275 CD2 LEU 3528 1742 186 1689 12.494 45.618 1.000 13.60 ANISOU 1275 CD2 LEU 187 9.286 2608 -26 -95 137 1276 N SER MOTA 1234 187 1326 13.734 44.826 1.000 13.22 ANISOU 1276 N SER 187 9.388 2338 -54 -68 2 9 1277 CA SER MOTA 1197 187 1489 ANISOU 1277 CA 44.134 1.000 12.79 SER 187 10.736 13.853 2192 -17 -114 - 9 0 SER 1278 C MOTA 1186 44.356 1.000 14.50 187 1482 ANISOU 1278 C SER 187 11.683 13.076 SER 76 -224 -113 MOTA 1279 0 2720 187 1532 1257 45.811 1.000 12.87 SER ANISOU 1279 O 14.915 187 9.201 1280 CB -154 9 8 SER ATOM 164 2147 187 1463 1282 SER 46.716 1.000 13.22 ANISOU 1280 CB 187 10.296 14.873 -143 2 2 4 SER 1281 OG 2015 -34 1420 187 1589 ANISOU 1281 OG SER

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	_		- 55 -		000 13 44
ATOM 1282 N	MET 188	3 10.898	14.844	43.292 1.	000 13 · 4 <u>4</u> ; <u>4</u> -34 -26
ANISOU 1282 N	MET 188	3 1552	1334	2221 -6	000 12.11
ATOM 1283 CA	MET 188	3 12.215	15.380	1833 29	-60 - 61
ANISOU 1283 CA	MET 188	3 1508	1261	1833 2-	000 12.78
ATOM 1284 C	MET 188	8 12.853	16.022	2136 1	57 -311 - 42
ANISOU 1284 C	MET 188	8 1563	1156	44 600 1	.000 13.40
ATOM 1285 0	MET 18	8 13.896	15.550	2294 1	16 -264 - 26
ANISOU 1285 O		8 1408	1390 16.300	41 667 1	.000 13.66
атом 1286 СВ	-	8 12.038	15.300	2123 4	4 -161 20/
ANTSOU 1286 CB		8 1565	17.095	41 315 1	.000 14.05
ATOM 1287 CG		8 13.296	1595	2046 6	6 150 1 3 3
ANISOU 1287 CG		8 1697 8 14.600	15.971	40.752 1	.000 14.96
ATOM 1288 SD		8 1565	1591	2529 1	09 -81 110
ANISOU 1288 SD		8 16.005	17.102	40.686 1	.000 17.74
ATOM 1289 CE	_	88 1852	2032	2855 -	242 505 121
ANISOU 1289 CE	MET 18 VAL 18	39 12.244	17.112	44.616 1	.000 12.62
ATOM 1290 N ANISOU 1290 N	VAL 18	39 1586	1203		03 -147 -134
		39 12.565	17.671	45.918 1	.000 12.60 -228 -11 - 44
		39 1412	1438	1937 -	-228 =11 -44
	VAL 18	39 11.285	17.968		1.000 11.71 -170 -171 - 49
ATOM 1292 C ANISOU 1292 C	VAL 18	89 1328	1294		-170 -171 - 4 9 1.000 12.56
ATOM 1293 0	VAL 1	89 10.227	18.099	46.050	21 -320 - 49
ANISOU 1293 O	VAL 1	89 1446	1291		1.000 12.95
ATOM 1294 C	R VAL I	89 13.440	18.955	2252	-174 -205 9 4
ANTSOU 1294 C		89 1150	1517 18.637	220	1.000 15.54
атом 1295 С		89 14.778	2094	2127	-140 161 9 ¹
ANTSOU 1295 C		89 1376		~	1.000 15.00
ATOM 1296 C		89 12.73(89 1763	1391	2547	-130 - 483 8 1
ANISOU 1296 C		90 11.42			1.000 12.18
ATOM 1297 N		90 1445	1422	1760	-109 -130 1 0
ANISOU 1297 N ATOM 1298 C	_	90 10.35	3 18.454		1.000 11.98 -57 -221 -151
ATOM 1298 C ANISOU 1298 C		90 1292	1356	1003	-57 -221 -151
		190 10.87	9 19.63	0 49.710	1.000 12.47
ATOM 1299 C ANISOU 1299 C	THR 1	190 1178	1436	2124	-32 -297 - 232 1.000 15.06
ATOM 1300 (THR 3	190 11.95	9 19.52		46 -571 -446
ANISOU 1300 (THR ?	190 1424	1767	2531	1.000 13.16
атом 1301 (CB THR	190 9.913	17.29		-168 80 -121
ANTSOU 1301 (CB THR	190 1509	1605 16.20		1 000 14 47
атом 1302 (OG1 THR	190 9.481	1460	2334	-100 -25 -194
ANISOU 1302	00=	190 1693		3 50.734	1.000 14.79
атом 1303	CG2 THR	190 8.778 190 1696	1510	2415	13 230 - 0 2
ANISOU 1303		191 10.14			1.000 12.97
ATOM 1304		191 1329	1449	2119	23 -21 - 286
ANISOU 1304 ATOM 1305		191 10.5		os 50.526	5 1.000 13.75 78 -206 -301
		191 1543	1442	2238	
ANISOU 1305 ATOM 1306		191 9.60	3 21.9	64 51.76	3 1.000 14.47 83 -179 -412
ANISOU 1306		191 1543	. 1689	2265	5 1.000 16.58
ATOM 1307		191 8.37	0 21.8	68 51.64	219 -176 - 725
ANISOU 1307		191 1517	2486	2297	2 1 000 15 . 37
ATOM 1308	CB LEU	191 10.3		2680	58 -106 - 109
ANISOU 1308	CB LEU	191 1717 191 11.7			3 1.000 16.10
ATOM 1309	CG LEU	191 11.7		2680	-128 -113 -133
ANISOU 1309	CG LEU	191 1747		65 47.90	6 1.000 16.67
	CD1 LEU	191 2034	2093	2209	-23 -64 1 2
	CD1 LEU	191 11.5		59 48.35	0 1.000 18.53
ATOM 1311 ANISOU 1311	CD2 FER	191 229	7 1906	2837	-345 -437 1 4 8 -6 1 000 15 36
AN1SOU 1311 ATOM 1312	N ILE	192 10.	199 22.1	L48 52.94	6 1.000 15.36
AION 1312					

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	-56 - 2152 2204 -47 -165 -164
ANISOU 1312 N ILE 192 1479	2132 2204 - 13
300M 1313 CA 1LE 134 3.41/	-304 - 1/3 - 200
TYTCOM 1313 CA ILE 192 1400	22 423 55 010 1 000 15 . 58
ATOM 1314 C ILE 192 9.092	1072 2251 -199 -254 -220
ANISOU 1314 C ILE 192 1090	23 691 55.381 1.000 17.20
3.1()M 1313 0 =	2449 2229 -307 -341 -274
AN 1500 1515 7 102 9 722	20.920 55.040 1.000 17.03
ATOM 1316 CB ILE 192 9.722 ANISOU 1316 CB ILE 192 2246	1958 2266 -52 325 2303
ANISON 1317 CG1 ILE 192 9.454	19.596 54.317 1.000 19.80 2010 2473 -71 128 -382
ANT SOU 1317 CG1 ILE 192 3040	2010 2473 71
2 TOM 1318 CG2 ILE 192 0.999	$\frac{1}{2}$ $\frac{1}$
ANTSON 1318 CG2 ILE 192 2270	10 207 55 235 1 000 31.57
2TOM 1319 CD1 1LE 192 3.420	2114 5222 -398 -1094 / 65
ANISOU 1313 GEN 193 8 625	24.172 55.249 1.000 17.04
A LOM ASSISTE	2185 2248 112 -366 - 3 0 1
AN1300 1323 102 9 680	25.291 56.201 1.000 17.70 2167 2824 -204 -186 -559
ATOM 1321 CA GLN 193 1737	2107 2021
3 mom 1322 C GLN 193 / · 0 9 0	222 222 211 -040
ANISOU 1322 C GLN 193 1882	2024 27 426 1 000 26.60
ATOM 1323 O GLN 193 7.062	2042 4197 -965 -110 5 4
ANISOU 1323 O GLN 193 2000	200 55 643 1 000 23 - /4
A 1 ()M	5200 3561 500 -98 -514
AN1300 1321 30 0 013	27.304 54.559 1.000 28.26 27.304 3689 656 209 0
ANTEON 1325 CG GLN 193 4664	2384 3007
2 mov 1326 CD GLN 193 8.330	701 4 111
ANTSOU 1326 CD GLN 193 2868	2943 53 588 1 000 45.31
ATOM 1327 OE1 GLN 193 / 193	$\frac{1}{2}$
AN 1300 132, 322 CIN 193 9 080	29.748 54.345 1.000 30.44
	2588 5368 418 1259 0 4
NTOM 1329 N GLN 194 8.241	25.259 58.645 1.000 22.04 25.258 2690 303 -368 - 83
NICON 1329 N GLN 194 2926	2758 2690 303 300 22 68
ATOM 1330 CA GLN 194 / . 303	2855 82 -230 -130
ANISOU 1330 CA GLN 194 3144	26 254 60 663 1 000 22 19
Alum 1331 3	2760 2856 117 -396 - 320
ANIBOO 1331 3 104 7 999	27.100 60.418 1.000 23.20 -4.11
ATOM 1332 O GLN 194 7.882 ANISOU 1332 O GLN 194 4041	2877 2679 -313 22 21
NOM 1333 CB GLN 194 8.40	,
ANISOU 1333 CB GLN 194 4455	- 2707 50 083 1 000 28 80
ATOM 1334 CG GLN 194 9.10.	2520 4305 576 -121 4 7 4
ANISOU 1334 CG GLN 194 3108 ANISOU 1335 CD GLN 194 10.2	96 22.332 60.962 1.000 31.97
	5384 3800 824 339 10.3
ANISON 1336 OF1 GLN 194 11.4	21 22.325 60.474 1.000 27.28 4189 3397 118 133 - 249
ANT COU 1336 OF1 GLN 194 2781	4189 3397 110 23 82
ATOM 1337 NE2 GLN 194 9.99	3050 3832 989 645 800
ANISOU 1337 NE2 GLN 194 3540	25 891 61.658 1.000 23.30
ATOM 1338 N THR 195 6.41	3387 -211 -235 - /20
AN 1500 1550 1	76 26.833 62.768 1.000 27.14
ANTCON 1339 CA THR 195 3459	3544 3308 25 -50 - 650
AN1300 1330 C THR 195 6.9	33 25.997 63.958 1.000 20.12 1.000
ANISOU 1340 C THR 195 382	5 2829 52 63 994 1 000 28.17
ATOM 1341 0 THR 195 6.6	2016 4815 481 1/1 -1030
ANISOU 1341 O THR 195 297	49 27.534 63.069 1.000 25.87
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ANISOU 1342 CB THR 195 342	



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- 58 --360 1601 -1460 4936 4375 200 4683 GLY ANISOU 1373 C 70.897 1.000 32.71 22.566 200 12.257 752 -1400 GLY -377 1374 0 4436 4072 200 3921 GLY 71.588 1.000 28.66 ANISOU 1374 O 21.939 201 10.264 463 - 326 1375 N PHE MOTA 145 2847 4229 201 3813 71.106 1.000 27.55 ANISOU 1375 N PHE 20.575 201 10.491 -233 219 -672 PHE 1376 CA MOTA ANISOU 1376 CA PHE PHE 1377 C -268 - 379 190 MOTA 2832 3682 201 2943 21.255 68.910 1.000 28.22 PHE ANISOU 1377 C 201 9.994 1378 0 PHE 10 -421 277 ATOM 3957 3184 201 3583 19.729 71.413 1.000 30.46 ANISOU 1378 O PHE 201 9.250 1379 CB PHE -371 -40 -73 3560 4862 201 3153 ANISOU 1379 CB PHE 18.262 71.027 1.000 34.89 201 9.425 1380 CG PHE 162 8 9 MOTA 4632 -772 201 4015 201 10.395 17.472 71.605 1.000 31.18 4609 ANISOU 1380 CG PHE 1381 CD1 PHE -93 -1105 -875 ATOM 4310 4103 4310 -875 -93 -17.681 70.078 1.000 28.84 201 3436 ANISOU 1381 CD1 PHE 201 8.613 1382 CD2 PHE 612 -107 329 MOTA 3960 201 2979 4019 ANISOU 1382 CD2 PHE 201 10.564 16.160 71.240 1.000 37.73 -1078 -1475 -500 1383 CE1 PHE MOTA 3608 4239 201 6489 ANISOU 1383 CE1 PHE 16.363 69.679 1.000 31.78 201 8.761 250 119 1384 CE2 PHE 652 MOTA 3911 3838 201 4327 ANISOU 1384 CE2 PHE 15.606 70.265 1.000 29.78 201 9.755 6 -638 -849 1385 CZ PHEMOTA 4211 201 3705 3397 69.144 1.000 23.51 ANISOU 1385 CZ PHE 202 11.706 19.751 VAL -292 -1 -578 1386 N MOTA 2868 3392 VAL 202 2671 ANISOU 1386 N 67.706 1.000 26.37 1387 CA VAL 202 11.969 19.626 -667 57 -724 ATOM 2946 ANISOU 1387 CA VAL 202 3025 4050 67.198 1.000 22.75 VAL 202 11.423 18.283 96 -120 -435 1388 C MOTA 2567 VAL 202 2729 3348 2567 96 -120 42 VAL 202 11.880 17.190 67.541 1.000 28.71 VAL 202 11.880 17.190 31.66 3348 ANISOU 1388 C VAL 1389 0 31 6 6 1 119 MOTA 3859 3799 202 3249 202 13.476 19.721 67.415 1.000 24.99 ANISOU 1389 O VAL ATOM 1390 CB VAL ANISOU 1390 CB VAL -278 283 152 3008 3427 202 3060 202 13.715 19.464 65.938 1.000 27.70 1391 CG1 VAL 87 1014 202 4642 2577 3307 87 1014 - 3 202 14.050 21.071 67.823 1.000 26.80 MOTA ANISOU 1391 CG1 VAL 474 - 398 1392 CG2 VAL -490 MOTA 202 2020 3000 3487 -490 474 - 203 10.405 18.402 66.333 1.000 24.10 3487 ANISOU 1392 CG2 VAL 1393 N SER -179 -528 MOTA 3356 3607 203 2194 17.231 65.940 1.000 23.70 ANISOU 1393 N SER 203 9.634 203 2373 -290 308 -533 1394 CA SER MOTA 3046 3584 203 10.168 16.511 64.710 1.000 21.28 203 2173 3041 2871 46 227 - 42 ANISOU 1394 CA SER SER 1395 C MOTA 203 10.159 15.285 64.640 1.000 27.60 SER ANISOU 1395 C -482 1010 -249 SER 1396 0 MOTA 3284 203 4105 3097 203 8.148 17.571 65.685 1.000 29.06 SER ANISOU 1396 0 -180 203 -2064 1397 CB SER 5001 3790 203 2251 18.175 66.843 1.000 32.55 ANISOU 1397 CB SER 203 7.584 1099 - 382 SER 920 1398 OG MOTA 4231 203 3840 4298 63.724 1.000 22.46 ANISOU 1398 OG SER 204 10.688 17.233 1399 N LEU 79 450 - 46 MOTA 3043 3013 LEU 204 2476 1400 CA LEU 204 11.166 16.530 62.544 1.000 20.26 ANISOU 1399 N MOTA 2831 204 2200 62.747 1.000 18.83 ANISOU 1400 CA LEU 204 12.595 16.038 204 2151 2528 LEU 1401 C 2477 -75 MOTA LEU 63.251 1.000 20.47 ANISOU 1401 C 204 13.443 16.783 -303 -195 4 0 4 LEU 1402 0 MOTA 3059 2386 204 2333 61.362 1.000 21.42 LEU ANISOU 1402 O 204 11.103 17.486 LEU 1403 CB -16 311 ATOM 2871 2548 204 2718 ANISOU 1403 CB LEU

- 59 -18.188 61.079 1.000 33.57 204 9.769 1404 CG LEU -1316 1172 MOTA 177 5617 204 2820 4319 ANISOU 1404 CG LEU 204 2820 4319 5617 17.000 36.19 204 9.797 18.747 59.660 1.000 36.19 1405 CD1 LEU 1276 -1167 987 5540 3807 204 4402 17.234 61.219 1.000 37.76 ANISOU 1405 CD1 LEU 204 8.581 -526 -1896 686 1406 CD2 LEU 5960 5328 ANISOU 1406 CD2 LEU 204 3058 205 12.864 14.836 62.284 1.000 20.33 2563 104 -31 -129 1407 N GLN MOTA 205 14.209 14.247 62.335 1.000 18.88 205 2522 2225 2425 -6 -181 3 6 205 14.512 13.504 61.036 1.000 18.19 205 1986 2383 2543 -143 -188 - 8 0 205 13.577 13.033 60.408 1.000 19.87 205 1974 3063 2514 -125 -212 - 23 2644 ANISOU 1407 N GLN 1408 CA GLN MOTA ANISOU 1408 CA GLN GLN1409 C ATOM ANISOU 1409 C GLNGLN 2514 -125 -212 - 237 1410 0 205 1974 3063 2514 -125 -212 -205 14.296 13.267 63.493 1.000 24.25 MOTA ANISOU 1410 O GLN1411 CB GLN -343 2 9 6 205 3948 2716 2548 202 -343 2 205 14.164 13.948 64.856 1.000 30.64 MOTA ANISOU 1411 CB GLN GLN-327 - 8 9 1412 CG 2382 850 205 4099 5159 2382 850 -327 - 3 205 14.744 13.078 65.948 1.000 28.28 ATOM ANISOU 1412 CG GLN3633 2640 -161 -1015 -390 1413 CD GLN ATOM 205 14.307 11.921 66.041 1.000 37.69 205 5733 5073 3515 -2145 -699 4 7 8 ANISOU 1413 CD GLN 1414 OE1 GLN MOTA ANISOU 1414 OE1 GLN 205 15.710 13.553 66.711 1.000 40.53 205 6798 4417 4185 -1341 -2865 3 2 3 1415 NE2 GLN MOTA ANISOU 1415 NE2 GLN 206 15.752 13.471 60.576 1.000 18.52 ALA 2769 -240 -13 4 1416 N ATOM206 2070 2199 ATOM 1417 CA ALA 206 16.152 12.700 59.405 1.000 18.42

ANISOU 1417 CA ALA 206 2074 2351 2575 -100 -158 2

ANISOU 1418 C ALA 206 17.343 11.802 59.738 1.000 17.41 2575 -100 -158 2 ALA 206 2107 2158 2350 -185 -254 - 3 ALA 206 18.123 12.203 60.613 1.000 20.67 ALA 206 2469 2410 2973 -48 -711 - 3 2350 -185 -254 - 17 ANISOU 1418 C 2410 2973 -48 -711 - 3 9 6 1419 0 MOTA ATOM 1420 CB ALA 206 16.637 13.599 58.270 1.000 18.77 ANISOU 1420 CB ALA 206 2119 2310 2703 156 -65 1 ATOM 1421 N GLU 207 17.492 10.764 58.931 1.000 18.09 ANISOU 1421 N GLU 207 2092 2101 2680 -249 -496 -ANISOU 1419 O 2703 156 -65 147 2680 -249 -496 -162 ANISOU 1421 N 1422 CA GLU -432 - 44 ATOM ANISOU 1422 CA GLU 220 -560 5 4 4 GLU 1423 C MOTA ANISOU 1423 C GLU GLU 1424 0 MOTA ANISOU 1424 O GLU -1226 6 1 GLU 1425 CB MOTA ANISOU 1425 CB ${ t GLU}$ GLU 93 4 6 7 1426 CG MOTA 207 20.730 7.791 57.129 1.000 31.69 ANISOU 1426 CG GLU 4134 -1218 -175 1 2 2 GLU 1427 CD MOTA 5178 207 2729 ANISOU 1427 CD GLU 55.943 1.000 26.97 207 20.376 7.611 1428 OE1 GLU 31 -256 309 MOTA 3404 3993 207 2849 ANISOU 1428 OE1 GLU 57.407 1.000 30.70 207 21.908 8.121 1429 OE2 GLU -233 -342 -1168 3416 5764 208 20.919 10.936 59.078 1.000 18.53 207 2484 ANISOU 1429 OE2 GLU 130 -362 3 2 0 VAL 1430 N MOTA 2907 VAL 208 2020 2112 1430 N VAL 208 22.150 11.547 58.541 1.000 19.53 ANISOU 1430 N 3137 39 -476 630 MOTA 2238 208 2044 208 23.341 10.755 59.088 1.000 21.95 ANISOU 1431 CA VAL 3507 225 -461 797 VAL 1432 C MOTA 2792 208 2040 60.314 1.000 23.82 ANISOU 1432 C VAL 208 23.460 10.663 3547 -40 -858 8 2 5 VAL 1433 0 MOTA 3240 208 2262 208 22.271 13.027 58.905 1.000 19.72 VAL ANISOU 1433 O 1434 CB VAL ATOM

ANISOU 1434 CB VAL 208 1918 2429 3145 -47 -308 3 1 1 ATOM 1435 CG1 VAL 208 23.524 13.626 38.291 1.000 23.14 2 ANISOU 1435 CG1 VAL 208 25.524 13.626 38.291 1.000 23.14 2 ANISOU 1436 CG2 VAL 208 21.030 13.812 38.469 1.000 19.47 5 ANISOU 1437 N GLY 209 24.80 24.48 24.9 4123 46.5 -711 3 6 ANISOU 1437 N GLY 209 25.00 24.80 24.49 4123 46.5 -711 3 6 ANISOU 1437 N GLY 209 25.00 29.8 3 9.9 37.4 58.773 1.000 26.48 7 ANISOU 1438 CA GLY 209 25.30 6 3.59 4450 440 440 0 GLY 209 29.8 3 9.9 3 9.9 450 460 -487.5 16 ANISOU 1443 PC GLY 209 29.5 6.00 9 7.835 60.629 1.000 30.01 1.45 ANISOU 1441 N GLY 210 23.691 7.702 59.523 1.000 26.6 4 ANISOU 1442 CA GLY 210 23.691 7.702 59.523 1.000 26.6 6 5 5 0 ANISOU 1442 CA GLY 210 23.263 6.585 60.360 1.000 29.77 8 4 ANISOU 1443 PC GLY 210 23.263 6.585 60.360 1.000 29.77 8 4 ANISOU 1444 O GLY 210 23.263 6.585 60.360 1.000 29.77 8 4 ANISOU 1443 PC GLY 210 24.663 3 091 369 -55 ANISOU 1445 N ALA 211 22.512 8.274 ANISOU 1445 N ALA 211 21.828 8.600 3.824 1.000 31.43 ANISOU 1446 CA ALA 211 3993 5984 ANISOU 1447 C ALA 211 21.828 8.600 3.825 1.000 30.13 5.62 ANISOU 1447 C ALA 211 21.828 8.600 3.825 1.000 31.43 ANISOU 1446 CA ALA 211 31.806 4 ANISOU 1448 O ALA 211 31.864 ANISOU 1449 CB ALA 211 31.849 ANISOU 1449 CB ALA 211 31.849 ANISOU 1447 C ALA 211 21.849 ANISOU 1448 O ALA 211 31.849 ANISOU 3449 CB	WO 00/23004	PC 1/G II 7 GI S S S S
ANISOU 1434 CB VAL 208 1918 2429 3145 -47 -305 3 1 4 ATOM 1435 CG1 VAL 208 23 524 2374 3895 -202 284 3 4 9 ANISOU 1435 CG1 VAL 208 2524 2374 3895 -202 284 3 4 9 ANISOU 1436 CG2 VAL 208 2462 279 2658 232 -667 - 57 ANISOU 1436 CG2 VAL 208 2462 279 2658 232 -667 - 57 ANISOU 1437 N GLY 209 2500 2449 4123 465 -7711 3 6 ANISOU 1437 N GLY 209 2500 2449 4123 465 -7711 3 6 ANISOU 1437 N GLY 209 2500 2449 4123 465 -7711 3 6 ANISOU 14438 CA GLY 209 1887 3599 4450°, 460 -487 5 1 6 ANISOU 1449 C GLY 209 3469 3240 4693 238 -1422 7 3 2 ANISOU 1440 O GLY 209 4053 4488 348 1225 -887 8 3 ANISOU 1440 O GLY 209 4053 4488 348 1225 -887 8 3 ANISOU 1441 N GLY 210 2460 3091 361 361 442 CA GLY 210 2460 3091 361 361 442 CA GLY 210 2460 3091 3619 -55 -997 8 4 ANISOU 1440 CA GLY 210 22 622 632 639 3 619 -55 -997 8 8 ANISOU 1440 CA GLY 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 210 22 622 625 6187 62 ANISOU 1444 O GLY 210 4152 6516 5082 2187 4 -67 23 4 6 ANISOU 1444 O GLY 210 4152 6516 5082 2187 4 -67 23 4 6 ANISOU 1445 O ALA 211 22 512 8 674 6 ANISOU 1445 O ALA 211 22 512 8 674 6 ANISOU 1445 O ALA 211 22 622 627 6 ANISOU 1445 O ALA 211 22 622 632 638 63 225 1 000 38 22 8 ANISOU 1445 O ALA 211 22 622 637 6 ANISOU 1445 O ALA 211 22 812 8 ANISOU 1445 O ALA 211 21 2828 ANISOU 1445 O ALA 211 21 2812 ANISOU 1445 O ALA 211 21 2812 ANISOU 1445 O ALA 211 21 2812 ANISOU 1445 O ANISOU 1445	WU 99/33994	- 60 -
	ANTSOU 1434 CG VAL 208 23.524 ANTSOU 1435 CG1 VAL 208 25.24 ANTSOU 1436 CG2 VAL 208 24.20 ANTSOU 1436 CG2 VAL 208 24.20 ANTSOU 1437 N GLY 209 24.180 ANTSOU 1438 CA GLY 209 25.306 ANTSOU 1438 CA GLY 209 24.905 ANTSOU 1439 C GLY 209 24.905 ANTSOU 1441 N GLY 209 25.306 ANTSOU 1441 N GLY 209 25.609 ANTSOU 1441 N GLY 210 23.691 ANTSOU 1441 N GLY 210 23.691 ANTSOU 1442 CA GLY 210 23.691 ANTSOU 1443 C GLY 210 23.263 ANTSOU 1443 C GLY 210 23.263 ANTSOU 1444 O GLY 210 23.263 ANTSOU 1444 O GLY 210 22.622 ANTSOU 1445 N ALA 211 22.512 ANTSOU 1445 N ALA 211 22.512 ANTSOU 1446 CA ALA 211 20.663 ANTSOU 1448 O ALA 211 20.652 ANTSOU 1448 O ALA 211 20.663 ANTSOU 1448 O ALA 211 20.663 ANTSOU 1448 O ALA 211 3661 ANTSOU 1448 O ALA 211 20.665 ANTSOU 1449 CB ALA 211 20.652 ANTSOU 1445 CA ALA 211 3661 ANTSOU 1445 CA ALA 211 3661 ANTSOU 1445 CA ALA 211 3661 ANTSOU 1445 CA ALA 211 3644 ANTSOU 1445 CA ALA 211 3661 ANTSOU 1445 CA ALA 211 3644 ANTSOU 1445 CA ALA 211 3644 ANTSOU 1445 CA ALA 211 3661 ANTSOU 1451 CA PHE 212 19.68 ANTSOU 1451 CA PHE 212 19.68 ANTSOU 1453 O PHE 212 19.68 ANTSOU 1455 N THR 213 3644 ANTSOU 1455 N THR 213 3644 ANTSOU 1455 N THR 213 18.15 ANTSOU 1456 CA THR 213 3587 ANTOM 1456 CA THR 213 3587 ANTOM 1458 O THR 213 3155 ANTOM 1459 CB THR 213 3587 ANTOM 1459 CB THR 213 3582 ANTOM 1450 OG1 THR 213 3582 ANTOM 1450 OG1 THR 213 320.3 ANTSOU 1450 OG1 THR 213 320.3 ANTSOU 1450 CG THR 213 320.3 ANTSOU 1450 CG THR 213 3582 ANTOM 1450 CA ASP 214 2790 ANTSOU 1460 OG1 THR 213 3582 ANTOM 1450 CG THR 213 3582 ANTOM 1450 CG THR 213 320.3 ANTSOU 1463 CA ASP 214 2790 ANTSOU 1463 CA ASP 214 1	2429 3145 -47 -308 5 ± ± 13.626 58.281 1.000 23.14 2374 3895 -202 284 349 13.812 58.469 1.000 19.47 2279 2658 232 -667 -87 10.169 58.246 1.000 23.66 2449 4123 465 -711 3 9.374 58.773 1.000 26.42 3599 4450.9 460 -487 5 16 8.250 59.695 1.000 30.01 3240 4693 238 -1422 7 3 7.835 60.629 1.000 31.45 4458 3438 1225 -8978 3 7.702 59.523 1.000 36.66 3 3 3 4458 3438 1225 -8978 3 3 7.702 59.523 1.000 29.78 3 3091 3619 -55 -9975 58 4 6.187 62.481 1.000 32.81 4 4207 -2536 732 5 0 6.187 62.481 1.000 34.43 4 <
	MILOGO ZZZZZ	

WO 99/33994	- 61 -
	12 430 62 678 1 000 23 . 02
ATOM 1400 C ADI DII I	7093 3404 -167 -52 -572
ANISOU 1465 O ASP 214 17.205	18.058 65.637 1.000 23.54
ANTSOU 1466 CB ASP 214 3304	17 506 67 004 1 000 24 . 93
ATOM 1467 CG ASP 214 10.313	70=0 3079 450 -41/-614
ANISOU 1467 CG MS2 214 16 357	16.395 67.113 1.000 29.17
ATOM 1468 OD1 ASP 214 4134	3070 3878 202 -705 2 6 2 18.191 67.990 1.000 34.38
ATOM 1469 OD2 ASP 214 17.276	$\frac{1}{2040}$ $\frac{107}{1017}$ $\frac{-1413}{1017}$
ANISOU 1469 OD2 ASP 214 6917	19 452 62 859 1.000 20.74
ATOM 1470 N LEU 215 2426	2372 3081 86 -60 3 0 6
ATOM 1471 CA LEU 215 15.568	19.401 61.796 1.000 20.55 2013 2899 -202 -178 1 4 1
ANISOU 1471 CA LEU 215 2895	20 552 62.332 1.000 19.02
ATOM 1472 C LEU 215 14.724 ANISOU 1472 C LEU 215 2482	2240 2504 -142 -34 321
ANTOM 1473 O LEU 215 13.510	20.613 62.142 1.000 22.39 2483 3389 -160 -475 5 7 3
ANISOU 1473 O LEU 215 2635	10 722 60 650 1 000 22.04
ATOM 1474 CB LEU 215 14.828	2510 3086 -140 -261 - 63
ANISOU 1111	17.502 60.128 1.000 25.25
ANTSOU 1475 CG LEU 215 3680	16 726 50 174 1 000 27 . 12
ATOM 1476 CD1 LEU 215 14.000	2482 419 -1128 - 05
ANISOU 11.00 000 1011 015 16 881	18.046 59.510 1.000 30.76
ANTCOH 1477 CD2 LEU 215 3434	3089 5165 1003 524 501
ATOM 1478 N PRO 216 15.363	2101 2879 -157 148 1 0 3
ANISOU 1478 N PRO 216 2407 ATOM 1479 CA PRO 216 14.665	22.534 63.708 1.000 22.42
ANTSON 1479 CA PRO 216 2869	2812 2836 272 10 - 22 8
ATOM 1480 C PRO 216 14.201	3/33 3/86 566 -131 - 315
ANISOU 1480 C PRO 216 4118	23 759 61.586 1.000 24.67
ATOM 1481 O PRO 216 14.700 ANISOU 1481 O PRO 216 3682	2406 3284 187 -1/6 - 2 6
ATOM 1482 CB PRO 216 15.693	2010 2011 -210 110 -
ANISOU 1482 CB PRO 216 3108	22 701 64.146 1.000 28.31
ANT COU 1483 CG PRO 216 2994	2996 4766 -88 -117-1434
ATOM 1484 CD PRO 216 16.807	7 21.405 63.436 1.000 24.55 1777 5197 -436 -83 -348
ANISOU 1484 CD PRO 216 2353	. 24 207 63 102 1 000 24 . 13
ATOM 1485 N TVR 217 3237	2704 3229 244 -631 - 511
ANISON 1486 CA TYR 217 12.67	5 25.510 62.462 1.000 26.08 2899 4498 104 -592 3 9
ANISOU 1486 CA TYR 217 2514	4 26 516 62.369 1.000 25.24
ATOM 1487 C TYR 217 13.82 ANISOU 1487 C TYR 217 3049	2948 3592 -257 -506 - 536
ATOM 1488 0 TYR 217 14.57	0 26.675 63.340 1.000 31.78 2863 5096 -352 -2151 5 6 4
ANISOU 1488 O TYR 217 4114	2003 53 315 1 000 25.97
ATOM 1489 CB TYR 217 11.55 ANTSOU 1489 CB TYR 217 2747	7 2772 4346 86 -615 -16/
ATOM 1490 CG TYR 217 11.18	9 27.543 63.125 1.000 31.04 -6.44
ANTSOU 1490 CG TYR 217 3080	27 020 62 022 1.000 27.85
ATOM 1491 CD1 TYR 217 10.43	5314 511 -1/5 9 3
ATOM 1492 CD2 TYR 217 11.51	12 28.522 64.069 1.000 38.49 -749
ANTSOU 1492 CD2 TYR 217 4721	2813 7093 -880 1002
ATOM 1493 CE1 TYR 217 10.0	5/96 -41 10/ 6 9
ATOM 1494 CE2 TYR 217 11.1	13 29.835 63.827 1.000 42.90
ANISOU 1494 CE2 TYR 217 7112	2347 6842 -1413 -1513
ATOM 1495 CZ TYR 217 10.3	73 30.168 62.712 1.000 34.93

WO 99/33994	00
_	-62- 2747 6483 -1462 -545 1 6 6
ANISOU 1495 CZ TIR ZII Z	27 406 62 473 1 000 36.41
ATOM 1496 OH TYR 21/9.990	-2000 = 5439 = -753 = -250 = -209
ANISOU 1496 OH TYR 217 5499 ANISOU 1497 N ARG 218 14.022	27 110 61.218 1.000 25.58
A 1 () 1	2406 3852 -227 -533 -470
ANI300 1431 - 320 210 14 923	28 243 61.049 1.000 29.26
Δ1()(1 ± ± 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	3270 4219 -784 -1349 200
ANISOU 1130 01 200 210 14 113	29.336 60.365 1.000 24.81 29.348 2415 -382 -228 - 56
ATOM 1499 C ARG 218 4063	2343 2413
ATOM 1500 O ARG 218 13.746	
ANISOU 1500 O ARG 218 6298	2267
ATOM 1501 CB ARG 218 10.102	$\frac{1}{2}695$ 6732 -624 -703896
ANISOU 1501 CB ARG 218 3223	28 665 60.661 1.000 51.38
A 1 ()(1)	-6760 9015 -3031 430 -183
ANISOU 1301 12 12 210 19 539	28.606 59.701 1.000 38.84
ATOM 1503 CD ARG 218 4968	6308 3482 -3596 -1165 1647
ANISOU 1503 UE ARG 218 19.343	27.395 59.905 1.000 45.09 7495 4982 -2325 -962 - 94
ANT COU 1504 NE ARG 218 4655	1333 60 050 1 000 55.53
ATOM 1505 CZ ARG 218 20.272	27.208 58.959 1.000 55.53 11458 4340 -2701 -1188 -1948
ANTSOU 1505 CZ ARG 218 5299	22150 50 031 1 000 60 . 85
ATOM 1506 NH1 ARG 218 20.209	$\frac{1}{1}$
AN1500 1500 150 210 21 060	55 155 50 001 1 000 60 . 37
ATOM 1507 NH2 ARG 218 21.060 ANISOU 1507 NH2 ARG 218 8580	10111 4247 -2152 639 -4241
ANISOU 1307 170 210 13 971	30.496 60.972 1.000 25.89 4126 3086 35 296 -1014
ATOM 1508 N PRO 219 2625	4126 3086 33 290 132
ATOM 1509 CA PRO 219 13.003	2120 4730 -410 379 -696
ANISOU 1509 CA PRO 219 2828	31 959 58 981 1.000 28 . 43
ATOM 1510 C PRO 219 13.636	2010 4653 -190 116 -320
ANIBOO 1511 C DDO 219 12 904	4 32.393 58.081 1.000 34.17
ATOM 1511 O PRO 219 4734	3500 4/50 302 70
NTOM 1512 CB PRO 219 13.115	
ANISOU 1512 CB PRO 219 5621	3612 3032 629 1 000 42.38
ATOM 1513 CG PRO 219 13.30	5277 4688 -257 2084 -2080
ANIBOO 1511 CD DDO 219 14 37	0 30 943 62.289 1.000 32.77
A LOM	5719 2831 -602 820 -1003
ANISOU 1514 CD PRO 219 3901 ATOM 1515 N ASP 220 14.95	50 31.824 58.811 1.000 25.65 1582 4837 -276 801 -878
ANT CON 1515 N ASP 220 3328	1582 4837 -270 001
ATOM 1516 CA ASP 220 15.59	$\frac{1}{1}$ $\frac{1}$
ANISOU 1516 CA ASP 220 3594	21 205 56 451 1,000 28.46
AION 131.	5423 -111 1638 - 943
AN 1500 151.	32 31.620 55.433 1.000 25.80
ANTSON 1518 0 ASP 220 3249	2021 4533 -140 023
NTOM 1519 CB ASP 220 LD. J.	118/-1/4
ANISOU 1519 CB ASP 220 2351	22 21 013 58 502 1.000 42.36
ATOM 1520 CG ASP 220 17.80	2521 9912 -812 230 -937
AN 1500 1525 320 17 4	84 31.170 59.423 1.000 37.00
ATOM 1521 OD1 ASP 220 17.4 ANISOU 1521 OD1 ASP 220 3154	4148 6757 -104 -410 -2001
AUCOM 1522 OD2 ASP 220 18.9	081 31.787 57.937 1.000 37.5 1 2.66
ANTSON 1522 OD2 ASP 220 2520	4700 6969 93 -024 -79
ATOM 1523 N ALA 221 15.2	3398 -252 671 -659
ANISOU 1523 N ALA 221 4148	595 29 016 55.596 1.000 19.17
AION 1011	- 10c0 3251 -52 -94 - 010
AN 1500 1521 5 27 221 14 5	551 27.996 55.479 1.000 18.60
ATOM 1525 C ALA 221 14.5 ANISOU 1525 C ALA 221 1920	
M1000 1011 0	

- 63 -27.852 56.415 1.000 26.47 221 13.763 -1307 894 -904 ALA 1526 0 MOTA 3289 2641 221 4127 ANISOU 1526 O ALA56.104 1.000 19.36 28.316 221 16.939 1527 CB ALA-537 -316 6 6 2969 2333 221 2054 ANISOU 1527 CB ALA54.313 1.000 17.35 222 14.490 27.385 VAL -101 -323 -154 1528 N MOTA 2661 222 2089 1841 ANISOU 1528 N VAL 26.276 54.083 1.000 17.45 222 13.556 VAL -417 1 9 1529 CA 3004 -66 MOTA 2004 222 1620 ANISOU 1529 CA 222 14.333 24.965 54.077 1.000 15.69 VAL VAL -269 -349 -324 1530 C 222 15.512 24.934 53.716 1.000 17.84 222 1658 1730 3390 -108 -194 4 222 12.822 26.433 52.747 1.000 19.60 222 2267 2202 2979 91 -666 -30 MOTA 2471 VAL ANISOU 1530 C VAL 3390 -108 -194 4 8 1531 0 MOTA ANISOU 1531 O VAL 1532 CB VAL 2979 91 -666 -304 MOTA ANISOU 1532 CB VAL 51.563 1.000 21.96 1533 CG1 VAL 222 13.781 26.363 -645 -182 ATOM 2977 250 ANISOU 1533 CG1 VAL 222 2252 3113 1534 CG2 VAL 222 11.730 25.411 52.490 1.000 22.44 -497 -898 4 4 ATOM 3067 223 13.789 23.892 54.621 1.000 16.30 ANISOU 1534 CG2 VAL 222 2923 -93 -532 1535 N LEU -239 ATOM 2706 1694 223 1792 223 14.407 22.575 54.579 1.000 15.91 ANISOU 1535 N LEU -297 - 333 1536 CA LEU 2503 -93 MOTA 1864 223 1679 ANISOU 1536 CA LEU 223 14.114 21.908 53.243 1.000 14.86 LEU -141 -322 -458 1537 C MOTA 1537 2773 223 1337 223 12.969 21.888 52.766 1.000 16.23 LEU ANISOU 1537 C 1538 0 LEU 70 -391 -281 MOTA 2132 2719 223 1317 ANISOU 1538 O LEU 55.761 1.000 19.97 223 13.829 21.779 -121 205 -212 1539 CB LEU ATOM 2901 1945 223 2740 55.882 1.000 23.01 ANISOU 1539 CB LEU 223 14.298 20.348 -375 -170 9 1 LEU 1540 CG ATOM 4205 223 2668 1871 ANISOU 1540 CG LEU 56.143 1.000 23.73 1541 CD1 LEU 223 15.797 20.322 3378 69 135 3 1 6 MOTA ANISOU 1541 CD1 LEU 223 2570 3067 56.979 1.000 35.71 223 13.492 19.668 223 2813 3296 1542 CD2 LEU 1116 2333 7459 525 MOTA ANISOU 1542 CD2 LEU 224 15.115 21.370 52.570 1.000 14.18 VAL -320 - 205 1543 N 2560 -28 ATOM1446 224 1383 224 14.956 20.627 51.330 1.000 14.52 VAL ANISOU 1543 N -323 -127 1544 CA VAL MOTA -23 1501 2431 224 1585 VAL VAL 224 15.320 19.160 51.561 1.000 13.59 ANISOU 1544 CA 23 -290 -251 1545 C ATOM 2178 1522 224 1464 224 16.442 18.861 51.981 1.000 15.38 ANISOU 1545 C VAL 0 -505 -374 VAL1546 0 224 1464 1558 2822 0 -505 -37 224 15.832 21.209 50.222 1.000 14.25 MOTA ANISOU 1546 O VAL 1547 CB -461 -108 VAL MOTA -60 2407 224 1402 224 15.685 20.443 48.906 1.000 16.63 1606 ANISOU 1547 CB VAL 2474 -159 -408 - 421 1548 CG1 VAL MOTA 224 15.575 22.687 50.040 1.000 16.40 2164 ANISOU 1548 CG1 VAL 1549 CG2 VAL 6 -509 8 7 MOTA 2863 1562 224 1807 225 14.340 18.299 51.299 1.000 13.49 ANISOU 1549 CG2 VAL -353 - 130 1550 N PHE -66 MOTA 2106 1526 225 1494 225 14.647 16.882 51.162 1.000 14.67 ANISOU 1550 N PHE ATOM 1551 CA PHE ANISOU 1551 CA PHE -115 -61 -283 2431 1505 225 14.756 16.533 49.675 1.000 14.27 225 1639 -260 - 194 PHE 100 1552 C MOTA 2352 1533 225 1536 225 13.858 16.876 48.893 1.000 16.25 ANISOU 1552 C PHE 1553 0 PHE -311 - 88 ATOM 296 2569 225 1604 2000 51.749 1.000 15.57 ANISOU 1553 O PHE 225 13.537 15.999 1554 CB PHE -46 2 4 2740 -25 1563 225 1613 ANISOU 1554 CB PHE 53.257 1.000 17.95 225 13.387 15.996 -650 -302 2 0 3 PHE 1555 CG MOTA 2666 2267 ANISOU 1555 CG PHE 225 1888 54.157 1.000 27.39 225 14.409 15.809 1556 CD1 PHE MOTA

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-910 -109≟ 900 ANISOU 1556 CD1 PHE 225 2740 4234 3431 -910 -1091 9
ATOM 1557 CD2 PHE 225 12.125 15.863 53.820 1.000 21.09
ANISOU 1557 CD2 PHE 225 2333 2765 2917 -166 399 -5
ATOM 1558 CE1 PHE 225 14.211 15.673 55.521 1.000 26.82
ANISOU 1558 CE1 PHE 225 3108 3657 3424 -1044 -1241 1
ATOM 1559 CE2 PHE 225 11.910 15.910 55.186 1.000 21.65
ANISOU 1559 CE2 PHE 225 2994 2414 2817 623 239 -3
ANISOU 1559 CE2 PHE 225 2994 2414 2817 623 239 -3 3431 -166 399 -527 3657 3424 -1044 -1241 1128 239 - 39 ANISOU 1559 CE2 PHE 225 12.958 15.787 56.078 1.000 28.82 226 1744 1740 2735 -222 -236 - 1 2 227 14.150 13.722 46.928 1.000 13.20 ANISOU 1566 SG ATOM 1567 N CYS 1567 N GLY 227 1388 1513 2113 -28 -293 - 2 1568 CA GLY 227 13.352 12.496 46.899 1.000 12.58 1568 CA GLY 227 1279 1631 1872 -83 -438 - 2 1569 C GLY 227 13.903 11.541 45.849 1.000 12.54 GLY-293 -290 ANISOU 1567 N 1872 -83 -438 - 255 MOTA ANISOU 1568 CA GLY ANISOU 1568 CA GLY 227 1279 1631 1872
ATOM 1569 C GLY 227 13.903 11.541 45.849 1.000 12.54
ANISOU 1569 C GLY 227 1518 1279 1965 15 -288 - 79
ANISOU 1570 O GLY 227 1630 1523 2008 51 -155 8 2
ANISOU 1571 N ALA 228 13.212 10.400 45.712 1.000 13.02
ATOM 1571 N ALA 228 1490 1306 2151 59 -204 - 161
ANISOU 1571 N ALA 228 1649 1155 1912 -68 -119 - 63
ANISOU 1572 CA ALA 228 1649 1155 1912 -68 -119 - 63
ANISOU 1573 C ALA 228 1566 1288 2016 97 -223 - 5
ANISOU 1573 C ALA 228 1566 1288 2016 97 -223 - 5
ANISOU 1574 O ALA 228 14.482 9.132 2004 26 -6 - 131
ANISOU 1575 CB ALA 228 12.714 8.121 45.058 1.000 14.56
ATOM 1575 CB ALA 228 1808 1366 ATOM 1576 N ILE 229 12.909 10.695 ATOM 1577 CA ILE 229 1340 1391 2441 -43 -289 2 73
ANISOU 1576 N ILE 229 1327 1364 ATOM 1577 CA ILE 229 1327 1364 ATOM 1578 C ILE 229 1327 1364 ATOM 1578 C ILE 229 14.938 11.746 ANISOU 1578 C ILE 229 14.938 11.746 ANISOU 1579 O ILE 229 14.938 11.746 ANISOU 1579 O ILE 229 14.938 11.746 ANISOU 1579 O ILE 229 14.938 11.746 ANISOU 1580 CB ILE 229 11.768 11.888 AI.100 13.17 -354 - 42
ANISOU 1580 CB ILE 229 11.768 11.888 AI.100 15.72 ATOM 1581 CG1 ILE 229 10.599 10.920 ANISOU 1581 CG1 ILE 229 12.040 12.674 39.808 1.000 14.19 ANISOU 1581 CG1 ILE 229 12.040 12.674 39.808 1.000 14.19 2298 76 -364 1 7 4 MOTA 1279 1965 15 -288 - 79 ATOM 1581 CG1 ILE 229 10.599 10.920 40.973 1.000 15.72

ANISOU 1581 CG1 ILE 229 1218 1936 2817 85 31 1 1 8

ATOM 1582 CG2 ILE 229 12.040 12.674 39.808 1.000 14.19

ANISOU 1582 CG2 ILE 229 1670 1425 2298 76 -364 1 7 4

ANISOU 1583 CD1 ILE 229 10.745 9.924 39.836 1.000 20.03

ATOM 1583 CD1 ILE 229 2129 1814 3667 -208 -385 - 488

ANISOU 1584 N ALA 230 14.877 12.575 42.353 1.000 13.38

ATOM 1584 N ALA 230 1252 1378 2454 -97 -176 7 4

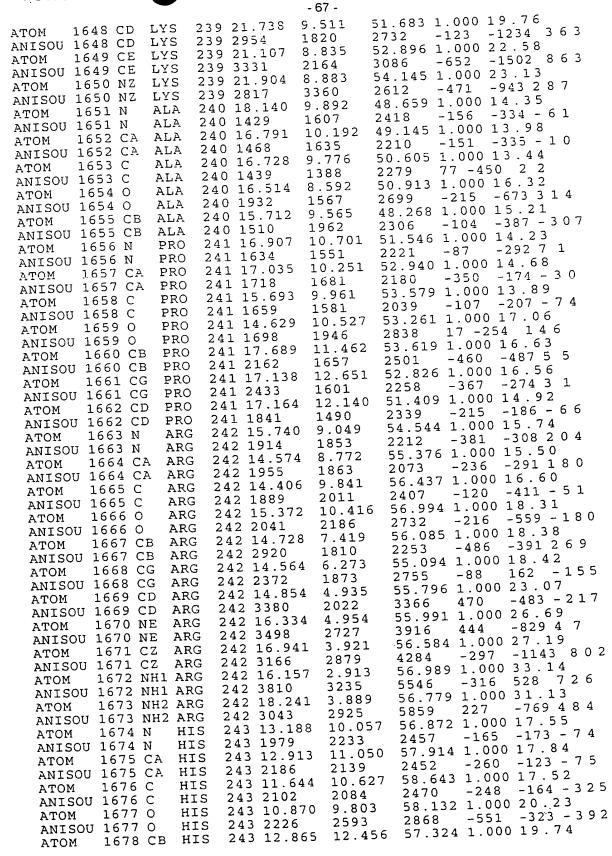
ANISOU 1585 CA ALA 230 16.209 13.185 42.130 1.000 12.30

ANISOU 1585 CA ALA 230 17.223 12.033 41.976 1.000 12.89

ANISOU 1586 C ALA 230 1491 1327 2079 128 30 - 20 2079 ALA 230 1491 1327 ANISOU 1586 C

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	_	- 65 -	41.146 1.000 13	. 65
ATOM 1587 0 A	LA 230 18.100	12.091	2418 108 4	4 6
	LA 230 1240	1530	43.345 1.000 13	
атом 1588 CB A	LA 230 16.588	3 14.000	2215 -186 -2	1 -229
ANISOU 1588 CB A	LA 230 1559	1415		3.31
атом 1589 N T	HR 231 17.14	3 10.978		- 1
ANTSOU 1589 N T	HR 231 1526	1318	42.659 1.000 1	3.32
атом 1590 CA T	THR 231 18.02	2 9.815 1307	2093 78 -302	3 2
ANISOU 1590 CA T	THR 231 1660	6 9.224	41.251 1.000 1	
ATOM 1591 C 7	THR 231 17.90			211 3
MMIDOG IOI	THR 231 1300		40 620 1.000 1	5.51
	THR 231 18.93 THR 231 1468	1759	2667 245 3	8 - 1 7 0
WMIDOG			43.688 1.000 1	3.03
		1302	2151 46 -166	1 2
ANIBOO TO			44.995 1.000 1	4.70
ATOM 1594 OG1		1614	2230 -99 3	2 - 14
ANISOU 1594 OG1 ATOM 1595 CG2			43.697 1.000 1	3.69
ATOM 1595 CG2 ANISOU 1595 CG2		1419	2225 113 -	211 1 9 /
	LEU 232 16.66	55 9.049	40.796 1.000 1	3.43 1 - 2.7
	LEU 232 1447	1384	2271 75 -404	1 - <i>2.</i> /
	LEU 232 16.4	16 8.396	39.527 1.000 1 2326 80 -468	. 4 . 1 1
	LEU 232 1809	1226	2326 80 -468	5 5 7
	LEU 232 16.9°	75 9.248	38.381 1.000 1 2376 209	-3 9 0
ANISOU 1598 C	LEU 232 1968	1557	2376 209 - 37.504 1.000 1	7 16
ATOM 1599 0	LEU 232 17.7	49 8.808		-116 - 519
ANISOU 1599 O	LEU 232 2024	1949	39.368 1.000	14.47
атом 1600 СВ	LEU 232 14.9	40 8.135 1630	2175 72 -39	6 -161
ANISOU 1600 CB	LEU 232 1692		38 155 1.000	15.89
ATOM 1601 CG	LEU 232 14.5		2329 120	-470 - 303
ANISOU 1601 CG	LEU 232 1941 LEU 232 15.1		30 202 1 000	23.19
ATOM 1602 CD1			3228 743	-1110 -851
ANISOU 1602 CD1			39 126 1 000	19.46
ATOM 1603 CD2			3126 -470	-523 - 6 6
ANISOU 1603 CD2 ATOM 1604 N	VAL 233 16.5		4 38.299 1.000	13./3
ATOM 1604 N ANISOU 1604 N	VAL 233 1736	1454	2025 -7 -26	1 2 9 3
ATOM 1605 CA	VAL 233 16.8	393 11.31	7 37.117 1.000	-73 1 0 7
ANISOU 1605 CA	VAL 233 167	1658	1926 141	1/ 08
ATOM 1606 C	VAL 233 18.	107 11.51	0 37.025 1.000	5 1 1 3
ANISOU 1606 C	VAL 233 171	1674		16.65
ATOM 1607 O	VAL 233 18.		2079 38 10	9 4 0 1
ANISOU 1607 O	VAL 233 192	3 2325	26 37.062 1.000	14.69
ATOM 1608 CB		098 12.62 $0 1696$	7 7 11 15 15 15 15 15 15 15 15 15 15 15 15	_
ANISOU 1608 CB	VAL 233 168		50 38 113 1.000	15.70
ATOM 1609 CG	1 VAL 233 16.		2698 34 15	6 - 2 8
ANISOU 1609 CG	1 VAL 233 161 2 VAL 233 16.			16.43
ATOM 1610 CG			2/59 251	117 590
ANISOU 1610 CG	THR 234 19.	_	94 38.175 1.000	14.23
ATOM 1611 N	THR 234 159		วกหว 146	-110 2 3 3
ANISOU 1611 N ATOM 1612 CA			08 38.148 1.000	71 / Q
ATOM 1612 CA ANISOU 1612 CA	·	1868	2602 63 -1	71 - 4 9
ATOM 1613 C	THR 234 21	346 10.6		211 - 51
ANISOU 1613 C	THR 234 17	L7 1865		17 25
ATOM 1614 O	THR 234 22	.558 10.6		200 229
ANISOU 1614 O	THR 234 17	76 1951		0 15.29
ATOM 1615 C	B THR 234 21	.030 12.6		-149 1 6 3
ANISOU 1615 C	B THR 234 16	67 1502		0 15.45
ATOM 1616 O	G1 THR 234 20	.849 11.8		59 4 4
ANISOU 1616 O	G1 THR 234 16	59 1708 .291 13.5	2303	0 16.61
ATOM 1617 C	G2 THR 234 20	.271 13.	J, 0	

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1613 CC2 MUD 23	A 156A 1672	3077 3 -34 - 42
ANISOU 1617 CG2 THR 23 ATOM 1618 N GLY 23	5 20.712 9.441	37.833 1.000 15.80
ANISOU 1618 N GLY 23	5 1905 1914	2564 193 29 - 219 37.792 1.000 17.10
ATOM 1619 CA GLY 23	3 22 1	2586 133 223 - 488
ANIBOO ICES	5 2049 1861 5 22.225 7.931	39.083 1.000 18.06
	5 2046 2049	2768 419 499 303
ATOM 1621 O GLY 23	55 23.285 7.289	39.010 1.000 21.26 3303 679 343 - 74
ANISOU 1621 O GLY 23	35 2167 2606	3303 679 343 - 74 40.237 1.000 16.17
ATOM 1622 N GLY 23	36 21.602 8.149 36 1663 1901	2582 36 291 3 0 5
ANIBOO ACCE OF CIVING	36 22.080 7.673	41.520 1.000 17.27
ANTSON 1623 CA GLY 23	36 2135 1671	2754 225 28 2 2 9
ATOM 1624 C GLY 23	36 23.033 8.639	42.194 1.000 16.88 2644 204 100 222
ANISOU 1624 C GLY 23	36 1880 1890 36 23.692 8.272	2644 204 100 2 2 2 43.193 1.000 19.42
	36 23.692 8.272 36 2165 2399	2814 314 -90 419
ANISOU 1625 O GLY 23 ATOM 1626 N GLN 23	37 23.134 9.890	41.746 1.000 16.99 2957 213 -213 167
ANISOU 1626 N GLN 2	37 1647 1851	255.
ATOM 1627 CA GLN 2	37 24.074 10.849 37 1608 2004	2752 72 177 9 8
MILDOO TOTAL	37 23.481 11.604	43.483 1.000 15.64
ANTSOU 1628 C GLN 2	37 1404 2136	2402 231 -146 2 0 0
ATOM 1629 0 GLN 2	37 24.183 12.382	44.164 1.000 18.17 2817 -227 -6 -46
ANIBOO III	37 1581 2508 37 24.456 11.855	41.217 1.000 17.17
	37 1912 2080	2532 71 141 - 7
ATOM 1631 CG GLN 2	237 25.304 11.221	
ANISOU 1631 CG GLN 2	237 1850 2410 237 25.721 12.302	2 7 2
	237 25.721 12.302 237 1680 2833	2979 104 317 30/
	237 26.602 13.110	39.436 1.000 24.27
ANTSOU 1633 OE1 GLN 2	237 1841 3145	=43.
	237 24.986 12.399 237 2007 2298	2735 432 374 202
ANISOU 1634 NE2 GLN 2 ATOM 1635 N VAL 2	238 22.221 11.359	43.807 1.000 14.75
ANTSOU 1635 N VAL	238 1563 1804	2237 -32 -54 4 3 44.862 1.000 14.41
ATOM 1636 CA VAL	238 21.533 12.075 238 1535 1553	2388 0 -44 3 2
ANA BOO	238 1535 1553 238 20.861 11.060	45 781 1.000 13.56
	220 1414 1392	2346 82 55 - 149
ATOM 1638 O VAL	238 20.136 10.174	45.302 1.000 15.87 2737 -218 -285 - 22
ANISOU 1638 O VAL	238 1655 1639 238 20.467 13.061	1 44 309 1 000 14.73
AIOH 2000 0-	238 20.467 13.061 238 1817 1626	2152 35 -437 - 95
ATOM 1640 CG1 VAL	238 19.805 13.764	4 45.489 1.000 15.70 2510 174 -524 - 423
ANISOU 1640 CG1 VAL	238 1965 1490	2020 1 000 1 6 9 2
ATOM 1641 CG2 VAL	238 21.064 13.996 238 1862 1718	2812 -60 -378 4 4 4
ANISOU 1641 CG2 VAL ATOM 1642 N LYS	239 21.119 11.15	3 47.071 1.000 14.47
ANISOU 1642 N LYS	239 1704 1474	2318 14 -40 1 2
ATOM 1643 CA LYS	239 20.470 10.36 239 1460 1617	0 48.104 1.000 14.43 2406 106 -168 1 7 9
ANISOU 1643 CA LYS ATOM 1644 C LYS	239 1460 1617 239 19.048 10.85	2 48 409 1 000 14 . 82
ATOM 1644 C LYS ANISOU 1644 C LYS	239 1533 1456	2642 102 -53 2 3 2
ATOM 1645 O LYS	239 18.839 12.06	37 48.457 1.000 14.74 2318 158 -275 1 9 0
ANISOU 1645 O LYS	239 1841 1442 239 21.320 10.43	15 49 385 1 000 16 . 40
ATOM 1646 CB LYS ANISOU 1646 CB LYS	239 21.320 10.43	2527 243 -543 2 5 2
ATOM 1647 CG LYS	239 20.767 9.549	
ANISOU 1647 CG LYS	239 1954 1759	2614 -58 -781 2 4 4



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	-68- 2248 2482 -188 -106 8 3
ANISOU 1678 CB HIS 243 2770	2240 2402 - 1 200 22 50
ATOM 1679 CG HIS 243 11.922	
ANTSON 1679 CG HIS 243 3449	12 200 54 879 1.000 25.87
ATOM 1680 ND1 HIS 243 12.203	2575 2473 -609 -403 $= 3$
ANTSOU 1680 ND1 HIS 243 4700	22 024 56 172 1 000 29 . 11
7 TOM 1681 CD2 HIS 243 10.000	$\frac{1}{4490}$ 3348 121 -421 1630
ANISOU 1001 - 11 182	12.573 54.109 1.000 32.92
ATOM 1682 CEI HIS 243 11.102 ANISOU 1682 CEI HIS 243 5835	3672 3001 -1102 -1367 089
ANISOU 1683 NE2 HIS 243 10.214	13.012 54.875 1.000 36.95 4201 4119 1019 -2016 987
NTCON 1683 NE2 HIS 243 5719	4201 4117 1010
ATOM 1684 N HIS 244 11.43/	
ANTSOU 1684 N HIS 244 2523	10 801 60 649 1.000 20.83
ATOM 1685 CA HIS 244 10.302	2485 2628 171 251 2/2
AN 1500 1005 61 WEG 244 9 927	11 968 61.551 1.000 20.33
ATOM 1003	2969 2953 -31 -78 -273
ANISOU 1000 0 WTG 244 10 482	13.073 61.510 1.000 21.71
ATOM 1687 O HIS 244 2057	3418 2//4 -555 145
ANISOU 1688 CB HIS 244 10.714	9.557 61.468 1.000 24.38 2644 2553 -76 -390 441
11TCOU 1688 CB HTS 244 4066	2044 2333 1 000 20 34
ATOM 1689 CG HIS 244 II.039	2400 2113 696 -727 - 89
ANISOU 1689 CG HIS 244 4158 ANISOU 1689 ND1 HIS 244 13.132	. 2 268 1 000 32.35
	3808 548 -485 -850
AN 1500 1050 1150 244 11 929	3 10.391 63.609 1.000 25.21
ATOM 1691 CD2 HIS 244 2937	4137 2505 -373 45 2 1 3
ANISON 1692 CE1 HTS 244 13.88	7 9.531 63.312 1.000 31.71 4277 3613 1224 -749 -518
ANTSOU 1692 CE1 HIS 244 4157	3477
ATOM 1693 NE2 HIS 244 13.14	2517 2633 94 -82 4 9 4
ANISOU 1693 NE2 HIS 244 3165 ANISOU 1694 N VAL 245 8.890	11 687 62.349 1.000 23.87
A10H 2007	2110 2322 -251 531 -310
ANIBOO 1005 CD 1701 245 8 473	12.691 63.349 1.000 21.000
ANT CON 1695 CA VAL 245 2785	3770 2888 481 145
AUDOM 1696 C VAL 245 8.024	2550 2112 -289 1/9 8 9
ANISOU 1696 C VAL 245 3220	3336 54 969 1.000 27.98
ATOM 1697 0 VAL 245 8.023	1428 42 295 - 29
ANISOU 1697 O VAL 245 3120 ANISOU 1698 CB VAL 245 7.020	12 114 63 099 1.000 26.02
ATOM 1698 CB VAL 245 7.020 ANISOU 1698 CB VAL 245 2621	7400 3777 94 -103 - 303
ATOM 1699 CG1 VAL 245 6.586	6 14.114 64.161 1.000 28.06 3330 4614 159 746 -485
ANTSOU 1699 CG1 VAL 245 2/1/	3330 4014 13300 51
ATOM 1700 CG2 VAL 245 6.94	1200 4220 1264 -303 - 33
ANISOU 1700 CG2 VAL 245 3564	0 12 696 65,603 1.000 28.08
A 1 U 1	7 2707 2543 -850 250 254
ANIBOO 1.700 03 313 246 9 56	7 12.316 67.003 1.000 27.43
ATOM 1702 CA ALA 246 4363 ANISOU 1702 CA ALA 246 4363	3360 2/0/ 232 273 68
AN1300 1703 C ALA 246 8.35	6 12.740 67.833 1.000 3.21
ANISOU 1703 C ALA 246 4915	67 563 1 000 29 . 5 4
ATOM 1704 O ALA 246 7.77	
ANISOU 1704 O ALA 246 3522	319 13 010 67.542 1.000 30.33
AIOM 1703 C2	3949 3011 615 -221 -422
ATOM 1706 N ALA 247 8.04	48 11.958 68.849 1.000 34.03
ANTCOM 1706 N ALA 247 448	3 5156 3311 -1190 400
ATOM 1707 CA ALA 247 7.03	10 FC27 3189 -1215 315 5 1 5
ANISOU 1707 CA ALA 247 418	12 010 71 081 1 000 33 31
ATOM 1708 C ALA 24/ /.0	22 240 -200 LEST
ANISOU 1708 C ALA 247 541	-

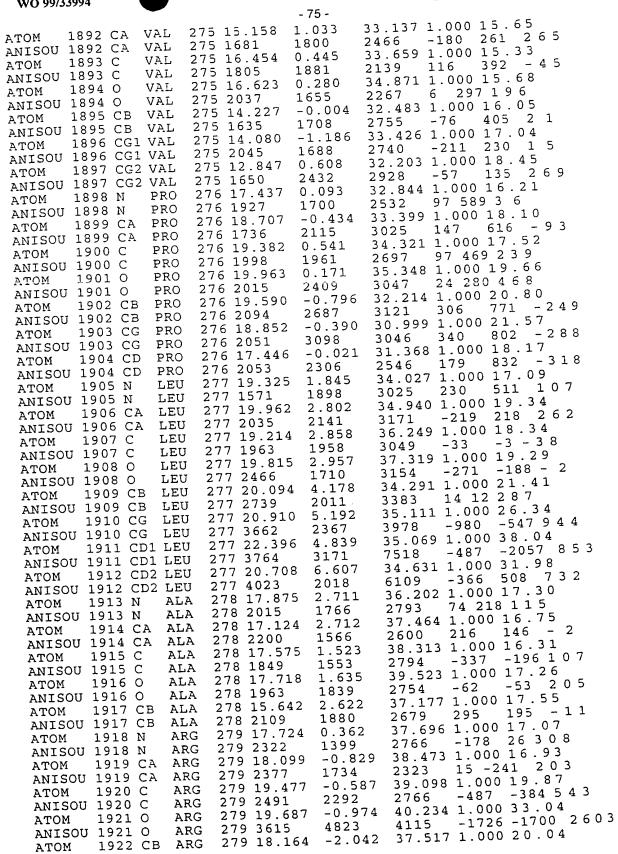
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ATOM 1709 O ALA 247 8.733 ANISON 1709 O ALA 247 5787	4470 4259 -378 -1519 1230
ANTISOU 1710 CB ALA 247 6.383	10.881 70.314 1.000 47.11
ANTSOU 1710 CB ALA 247 8374	0,20
ATOM 1711 N PRO 248 6.817	EASO 4836 -300 933 -97
ANISOU 1711 N PRO 248 5771 ANISOU 1711 CA PRO 248 7.256	14.581 72.773 1.000 44.85
ATOM 1712 CA PRO 248 7.256 ANISOU 1712 CA PRO 248 7568	5478 3996 -645 1413 2 1 4
ANISOU 1712 C. PRO 248 7.161	13.618 73.948 1.000 49.25 5660 5075 -1446 552 985
ANISOU 1713 C PRO 248 7978	12 794 74 014 1.000 45.48
ATOM 1714 O PRO 248 6.251	5391 4237 -1127 2573 - 796
AN 1300 1711 - 300 340 6 196	15.674 72.897 1.000 49.75
ATOM 1715 CB PRO 248 8563	4816 5523 -513 1238 -138 15.053 72.299 1.000 50.89
ATOM 1716 CG PRO 248 4.973	5564 6545 -108 2210 -1064
ANISOU 1716 CG PRO 248 7228	14.272 71.114 1.000 44.69
ATOM 1717 CD PRO 248 5.489 ANISOU 1717 CD PRO 248 6395	4579 6006 937 953 -5//
ANISOU 1719 N ARG 249 8.109	13.683 74.883 1.000 48.76 6341 3045 -1317 1069 - 477
ANISOU 1718 N ARG 249 9141	12 702 76 024 1 000 55.51
ATOM 1719 CA ARG 249 /.865	6014 4156 -1098 895 566
AN 1500 1711 5 5 5 6 944	13.466 76.916 1.000 46.09
ANTSON 1720 C ARG 249 5561	8382 3568 -2484 -7 1237 12.915 77.831 1.000 56.25
ATOM 1721 O ARG 249 6.244	$\frac{1}{6360}$ $\frac{7}{433}$ $\frac{377}{1799}$ $\frac{3995}{3995}$
ANISOU 1721 O ARG 249 /5/2	12.459 76.721 1.000 55.24
ATOM 1722 CB ARG 249 9.177 ANISOU 1722 CB ARG 249 8950	7715 4326 705 2864 1270
ANISON 1723 CG ARG 249 9.915	11.278 76.110 1.000 71.04 7330 6779 1135 3707 6 2 2
ANISOU 1723 CG ARG 249 12881	10 203 77 165 1,000 72.89
ATOM 1724 CD ARG 249 10.403 ANISOU 1724 CD ARG 249 11721	7001 7984 2171 2723 4 0 9
ANTSON 1725 NE ARG 249 11.12	4 9.162 76.580 1.000 70.73 9977 8271 2362 2650 - 266
ANISOU 1725 NE ARG 249 8627	9977
ATOM 1726 CZ ARG 249 12.03	0.417 7942 2304 2153 ± 3.3
AN1300 1720 3211 3PC 249 12 29	7 8.893 78.521 1.000 89.50
ANTSOU 1727 NH1 ARG 249 22286	6161 5559 2013 1022 3
ATOM 1728 NH2 ARG 249 12.08	10062 10295 1004 3886 4 4 1
ANISOU 1728 NH2 ARG 249 5358 ANISOU 1729 N ALA 254 1.981	18.918 75.430 1.000 85.24
ANTICOU 1729 N ALA 254 15501	7922 8964 -4581 -1437 2347
ATOM 1730 CA ALA 254 2.287	20.081 76.257 1.000 76.35
ANISOU 1730 CA ALA 254 12510	75 489 1 000 60.91
ATOM 1731 C ALA 254 2.943 ANTSOU 1731 C ALA 254 8383	7 5710 9040 -506 2886 1312
ATOM 1732 O ALA 254 4.174	1 21.309 75.487 1.000 /2.3/
ANISOU 1732 O ALA 254 8056	8109 11332 1002 4333
ATOM 1733 CB ALA 254 3.20	$\frac{1}{2}$
AN 1500 1.50 CT V 255 2 20	0 22.108 74.846 1.000 54.40
ANTSON 1734 N GLY 255 8029	5451 /190 554 2522
ATOM 1735 CA GLY 255 2.88	1424 836 -921
ANISOU 1735 CA GLY 255 5181 ATOM 1736 C GLY 255 3.64	0 22.565 72.921 1.000 38.82
ANTSON 1736 C GLY 255 4227	4772 5749 557 702 -1301
ATOM 1737 O GLY 255 4.58	5715 -128 -130 -222
ANISOU 1737 O GLY 255 2978	34 21.387 72.509 1.000 37.29
ANT CON 1738 N SER 256 504	4594 4527 389 11 -853
ATOM 1739 CA SER 256 3.73	38 20.606 71.429 1.000 35.71
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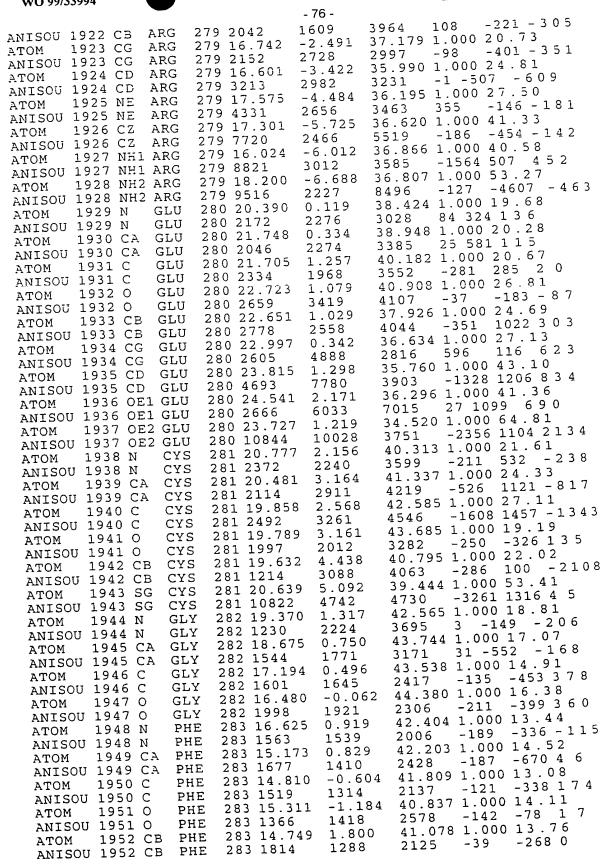
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ANISOU 1739 CA SER 256 4737	4533 4299 560 -501 -919 20.742 70.118 1.000 34.93
ATOM 1740 C SER 256 2.983	
ANT COLL 1740 C SER 256 4584	4000
ATOM 1741 O SER 256 3.251	
ANTSON 1741 O SER 256 3575	6107 3207 303
ATOM 1742 CB SER 256 3.845	111 / 117
ANISOU 1742 CB SER 256 3125	4030
ATOM 1743 OG SER 256 2.688	
ANISOU 1743 OG SER 256 298/	8497 11750 451 1943 2 6 3 0 21.700 70.030 1.000 3 5 . 5 4
ATOM 1744 N SER 257 2.065	5989 3479 347 242 - 86
ANISOU 1744 N SER 257 4037 ANISOU 1745 CA SER 257 1.379	21 993 68 767 1,000 30.95
AION III	5827 3109 170 672 - 509
AN1300 1713 011	22,538 67.760 1.000 30.63
AION 1.10	5524 2934 -476 765 -1297
AN1300 1717 O SER 257 3.359	23.159 68.199 1.000 34.70
ATOM 1747 O SER 257 3.335 ANISOU 1747 O SER 257 3500	6070 3616 -829 603 -1516
ATOM 1748 CB SER 257 0.331	23.088 69.036 1.000 30.70
ANT CON 1748 CB SER 257 3085	0310
ATOM 1749 OG SER 25/0.801	
ANISOU 1749 OG SER 257 8002	5175 11565 -999 -3375 363 22.384 66.471 1.000 30.51
ATOM 1750 N ARG 258 2.119	5068 2855 -332 677 -995
ANISOU 1750 N ARG 258 3668	22 819 65.396 1.000 28.15
A I OM	4620 2976 -106 358 -544
ANTEGO 2100 250 2 108	22.913 64.096 1.000 25.64
ATOM 1752 C ARG 256 2.196 ANISOU 1752 C ARG 258 3488	3381 2872 -676 273 -904
ATOM 1753 O ARG 258 1.132	22.294 63.981 1.000 24.93
ANTSON 1753 0 ARG 258 3162	3240 30,5 1 200 27 21
ATOM 1754 CB ARG 258 4.1/5	
ANISOU 1754 CB ARG 258 3158	20 500 64 570 1 000 30.90
ATOM 1755 CG ARG 258 3.861	2420 3531 -737 -738 -303
ANTEGO 1100 100 100 000 000 000 000 000 000 0	19 537 64.769 1.000 36.65
ATOM 1756 CD ARG 258 5.037 ANISOU 1756 CD ARG 258 5937	3466 4523 106 477 306
ATOM 1757 NE ARG 258 4.597	18.176 64.411 1.000 32.42 3858 5089 -85 -274 5 2 8
ANTSON 1757 NE ARG 258 3372	3858 5089 -85 -274 32 3
ATOM 1758 CZ ARG 258 4.633	3030 17.777 63.143 1.000 37.32 2958 5553 155 680 4 3
ANTSOU 1758 CZ ARG 258 5670	2930
ATOM 1759 NH1 ARG 258 5.0/5	150 311 - 103
ANISOU 1759 NH1 ARG 258 3077	16 566 62 824 1 000 38.66
	$\frac{1}{21}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{2}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{5}$ $\frac{1}{5}$
750 2 PT 750 2 PT 2 P	c 22 572 63 120 1,000 23 64
AION III	2570 2771 -519 315 -103/
ANISOU 1761 N THR 259 2625 ATOM 1762 CA THR 259 2.33	7 23.482 61.730 $1.000 21.97$
ANISOU 1762 CA THR 259 2614	2931 2800 -36 247 -101
ATOM 1763 C THR 259 3.52	8 23.197 60.808 1.000 19.76 2663 2587 -38 21 -699
ANTSON 1763 C THR 259 2257	2003
ATOM 1764 O THR 259 4.69	40E 10 + / 80
ANISOU 1764 O THR 259 2464	24 703 61 278 1 000 24 0 4
ATOM 1765 CB THR 259 1.68	$\frac{1}{2084}$ 3927 70 -157 -1229
ANISOU 1765 CB THR 259 2125	25 700 61 041 1 000 23 . 14
MION E. C. C.	$\frac{1}{1000}$
AN 1800 1.00 0.70	50 25.408 62.331 1.000 25.17
ANTSON 1767 CG2 THR 259 2941	$\frac{1}{1}$ 3229 3393 726 264 -130
ATOM 1768 N SER 260 3.23	34 22.706 59.600 1.000 20.41
ANISOU 1768 N SER 260 238	5 2762 2609 -61 74 -600
ATOM 1769 CA SER 260 4.2.	100 0 - 144
ANISOU 1769 CA SER 260 248	8 2459 2399 192 8 - 3 4 4

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ATOM 1824 NE AL	264 2151 264 2889 265 7.676 265 1192 265 7.900 265 1264 265 7.915 265 1266 265 1367 265 1367 265 9.246 265 1399 265 1399 265 1518 265 1518 266 1372 266 6.619 266 6.619 266 5.243 266 5.243 266 3.72 266 3.72 266 3.72 266 3.72 266 3.72 266 1351 266 3.72 266 1351 266 2.58 266 2.58	16.834 42.915 1.0 1283 2260 -10 19.730 43.156 1.0 1364 2019 -29 20.124 41.709 1.1 1399 2066 -2 21.314 41.318 1. 1546 1984 84 20.458 41.449 1. 1593 2197 -2 17.249 41.996 1. 1127 2043 -2 15.913 41.488 1. 1201 2012 -2 15.965 39.972 1. 1315 1948 29 16.860 39.396 1. 1318 2214 5 15.370 41.994 1 1477 2302 -2 15.606 43.488 1. 1686 2207 -1 15.606 43.488 1 1686 2207 -1 15.606 43.488 1 1686 2207 -1 15.606 43.488 1 1686 2207 -1 15.606 43.488 1 1686 2207 -1 15.606 43.488 1	-42 8 00 12.55 -120 4 6 00 12.39 4 -42 6 3 00 13.97 0 13 12 1 00 17.07 2 -410 4 9 7 00 17.41 0 433 1 1 2 00 20.59 6 -425 7 2 5 00 22.51 7 106 5 5 3 00 20.88 6 -22 3 0 6 00 11.81 7 47 1 9 00 12.01 03 16 -6 3 000 12.10 07 -81 3 000 12.10 07 -81 3 000 12.10 07 -81 3 000 12.19 92 -248 3 0 2 000 13.29 000 13.29 000 13.14 34 41 -2 0 000 12.06 000 12.06 000 12.06 000 12.06 000 12.06 000 12.07
ATOM 1818 CA AR ANISOU 1818 CA AR ATOM 1819 C AR ANISOU 1819 C AR ANISOU 1820 O AR ANISOU 1820 O AR ANISOU 1821 CB AF ANISOU 1821 CB AF ANISOU 1822 CG AF ANISOU 1822 CG AF ANISOU 1823 CD AF ANISOU 1823 CD AF ANISOU 1823 CD AF	G 266 6.586 G 266 1372 G 266 6.619 G 266 6.032 G 266 1430 G 266 5.243 G 266 5.243 G 266 1351 G 266 3.723 G 266 1369	1201 2012 -2 15.965 39.972 1. 1315 1948 29 16.860 39.396 1. 1318 2214 5 15.370 41.994 1 1477 2302 -2 15.606 43.488 1 1686 2207 -2 15.041 43.993 1 1362 2094 6	258 0 8 0 .000 11.75 9 -267 142 .000 13.06 -173 281 .000 12.95 189 43 - 33 .000 13.80 159 66 -115 .000 12.70 6 -22 8 4 .000 12.97
ANISOU 1824 NE ANISOU 1825 CZ ANISOU 1825 CZ ANISOU 1826 NH1 ANISOU 1826 NH1 ANISOU 1827 NH2 ANISOU 1827 NH2 ANISOU 1828 N PANISOU 1828 N PANISOU 1829 CA PANISOU 1829 CA PANISOU 1829 CA PANISOU 1829 CA PANISOU 1830 C	RG 266 1343 RG 266 1.30 RG 266 1432 RG 266 0.99 RG 266 1802 RG 266 0.30	1155	2 -165 -137 .000 11.34 .5 -149 -103 .000 13.39 .11 -38 7 2 .000 12.55 .25 -357 -159 .000 12.74 .000 12.74 .000 13.88 .000 13.88 .000 13.88 .000 13.88

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_	-73 - 8 14.155 37.772 1.000 13.60
ATOM 1831 0 PRO 267 4.99	160 118 9 1
ANTSOU 1831 O PRO 267 1648	13 761 27 509 1 000 15.30
ATOM 1832 CB PRO 26/ 6.2-	$\frac{1}{1240}$ $\frac{1}{2637}$ $\frac{1}{15}$ $\frac{-28}{15}$
ANISOU 1832 CB PRO 267 143	10 046 38 764 1 000 15 . 82
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ANISOU 1000 00 DDO 267 7 8	13.746 39.965 1.000 14.73
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AN1300 1031 05 3 9	33 15.051 35.939 1.000 13.27 1.27
ANTSON 1835 N ASN 268 160	1 1665 1/// -120 -45 121
700M 1836 CA ASN 268 4.0	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
ANTSOU 1836 CA ASN 268 179	3 1401 2020 1 000 13 14
ATOM 1837 C ASN 268 4.7	$\frac{1}{2}$ 1350 2156 -213 104 5 4
ANTSOU 1837 C ASN 268 148	12 467 34.934 1.000 13.90
ATOM TOO TOO	2167 -91 123 - 30
ANISOU IOSO O	15.338 33.690 1.000 15.74
AION TODO	$\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{3}$
ANISO 1840 CG ASN 268 5.0	11 16.862 33.811 1.000 13.11 7
ANTEON 1840 CG ASN 268 225	$\frac{1439}{55}$ $\frac{2162}{1000}$ $\frac{217}{75}$
ATOM 1841 OD1 ASN 268 4.	
ANTSOU 1841 OD1 ASN 268 25	73 17 502 33 319 1,000 16.61
ATOM 1842 ND2 ASN 268 6.	25/6 -50 -5/ 14 ⁴
ANISOU 1842 ND2 ASN 268 24 ANISOM 1843 N ALA 269 3.	531 12.712 34.594 1.000 13.99
AION TOTAL	$\frac{1}{77}$ 1467 2172 $\frac{-356}{100}$ $\frac{-65}{100}$
ANISOU IOIL ATA 260 3	278 11.286 34.353 1.000 13.42
ANT CON 1844 CA ALA 269 14	59 1405 2234 2206 113 93
AROM 1845 C ALA 269 4.	160 -5 (5)
ANISOU 1845 C ALA 269 12	33 318 1 000 14 . 97
ATOM 1846 O ALA 269 4.	2494 -143 112 8 8
AN1300 1010	806 11.051 34.008 1.000 13.76
ATOM 1847 CB ALA 269 1 ANISOU 1847 CB ALA 269 1	300 1474 2454 -60 -61 123
ANTISOU 1848 N ASP 270 4	.482 11.541 32.251 1.000 14.55 1.482 151 30 -5
ANTCOM 1848 N ASP 270 1	588 1476 25 300 1 000 14 83
ATOM 1849 CA ASP 270 5	$\frac{1}{1}$
ANISOU 1849 CA ASP 270 I	740 11 287 31 227 1.000 15.68
ATOM 1850 C ASP 270 6	2357 -224 143 8 9
AN1300 1030 C 30D 270 7	183 11.008 30.255 1.000 17.12
ANT CON 1851 0 ASP 270 1	952 2354 2200 -80 17 67
AM1500 1852 CB ASP 270 4	.718 11.681 29.800 1.000 17.51 319.126
ANISOU 1852 CB ASP 270 2	461 1966 22 649 1 000 18.22
ATOM 1853 CG ASP 270 4	2613 -88 -80 4 / 4
ANISOU 1853 CG ASP 270 2	396 13 826 30.607 1.000 20.55
	$\frac{1}{1}$
ANISOU 1031 02	1 646 13.698 28.552 1.000 23.60 12
ANT CON 1855 OD2 ASP 270	$\frac{2727}{2719}$
ADOM 1856 N PHE 2/1	7 2 2 2 2 2 4 1 7 9 7 3 1 4 1
ANISOU 1856 N PHE 271	1330 13132 22 644 1 000 14 4 1
AIOII = 00 · · · ·	2420 2423 110 29 2 0 3
ANIBOO 1031	9 275 10.349 32.325 1.000 13.31
ATOM 1858 C PHE 271 ANISOU 1858 C PHE 271	1402 1430 2225 -30 28 2 1 8
AN1500 1050 PHE 271	8.790 9.340 32.870 1.000 14.51 9.2
ANISOU 1859 O PHE 271	1900 1374 2392 -20 25 57
ATOM 1860 CB PHE 271	2/95 -66 -36 9
ANISOU 1860 CB PHE 271	1700 1721 2495 -66 336 10.386 11.791 34.516 1.000 14.56
ATOM 1861 CG PHE 271	10.300 11.72

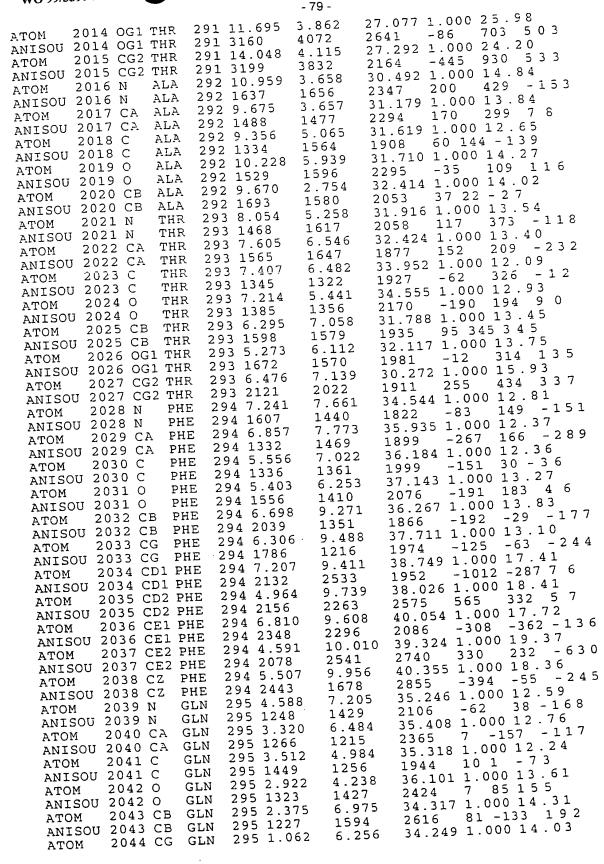
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7 TOM 1862 CD1 PRE 2/1 11.		-2.452 -2.35 -2.45
ANISOU 1002 022 271 10	.698 10.972	35.570 1.000 18.04 3130 -95 -540 172
ATOM 1863 CD2 PHE 271 218	82 1543	3130 -95 -540 1 / 2 34.166 1.000 17.54
ATOM 1864 CEL PHE 2/1 12	.786 12.092 38 1700	3128 -291 114 - 50
ANISOU 1864 CE1 PHE 2/1 16		35.899 1.000 18.84
	35 1646	3578 -392 -396 4 2 3
AN1300 1866 CZ PHE 271 13	.039 11.154	35.162 1.000 17.25 2415 -486 -19 -394
ANTSOU 1866 CZ PHE 271 24	44 1697 .278 10.298	2415 -486 -19 -394 31.453 1.000 13.78
ATOM 1867 N THR 2/2 10		2083 30 19 1 5 4
ANISOU 1007 1		30.938 1.000 13.99
ATOM 1868 CA THR 272 15	51 1660	2105 -99 83 6 7
ANISOU 1869 C THR 272 12	2.246 8.841	31.410 1.000 14.71 2441 -3 108 3 5 7
ANISOU 1869 C THR 272 1	598 1549 3.046 9.808	31 424 1 000 16 23
ATOM 1870 0 THR 2/21-		2780 - 246 5 185
ANISOO 1070 0 072 272 11	0.751 9.117	29.388 1.000 16.27 2119 191 125 8
ATOM 1871 CB THR 272 1	856 2205	2119 191 125 8 29.032 1.000 17.99
7TOM 1872 OG1 THR 2/2 3	.341 9.221 996 2473	2269 64 - 190 404
ANTSOU 1872 OG1 THR 2/2 I	1.249 7.856	28.723 1.000 17.94
	<u> </u>	2227 173 1// - 34
AN1300 1874 N PHE 273 1	2.567 7.600	31.743 1.000 14.91 2499 92 238 2 1 8
ANISOU 1874 N PHE 273 1	.644 1521 3.894 7.253	22 254 1 000 15.16
ATOM 1875 CA PHE 2/3 1		23/15 296 27/ 2 2
ANIBOO 1073 011 272 1	4.350 5.899	31.724 1.000 14.69
ATOM 1876 C PHE 273 1	L408 1647	2528 24 479 1 7 8 31.262 1.000 15.91
ATOM 1877 O PHE 2/3	13.541 5.086 1738 1767	25/1 -115 450 1 1
ANISOU 1877 O PHE 2/3	13.899 7.301	33.769 1.000 15.77
ATOM 1070 02	1758 1921	2314 - 344 286 123
ANISOU 1879 CG PHE 273	12.931 6.336	
ANTSON 1879 CG PHE 273	1390 1726 11.601 6.743	34 655 1.000 16.64
ATOM 1880 CD1 PHE 2/3		2521 -24 308 302
AN 1300 1000 022 DUE 273	13.295 5.038	34.7211.00015.23
ATOM 1881 CD2 PHE 273	1863 1624	2300
ATOM 1882 CE1 PHE 2/3	10.719 5.84° 1593 2158	2365 -162 294 144
ANTSON 1882 CEL PRE 2/3	1593 2158 12.419 4.14	8 35.354 1.000 16.01
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ANISOU 1884 CZ PHE 273	1843 2001 15.634 5.61	21 226 1 000 15.31
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ATOM 1886 CA SER 274	1476 1723	54 32 588 1 000 14.6/
ATOM 1887 C SER 2/4	15.953 3.28	- agac
ANISOU IOU, G	1 973 1877 1 16.310 3.4°	76 33.770 1.000 15.98
ANT COU 1888 O SER 274	1 1668 167	7 2728 126 143 133
ATOM 1889 CB SER 274	4 17.742 4.5	n 3110 735 940 /# 1
ANISOU 1889 CB SER 27	4 1487 201 4 18.362 3.2	80 31.334 1.000 18.03
ATOM 1890 OG SER 27	4 18.362 3.2 4 1839 196	1 2052 293 840 1 0 0
ANISOU 1090 00 00 00 00 00 00 00 00 00 00 00 00	5 15.395 2.1	33 32.182 1.000 15.30 1.000 1.000 15.30 1.000 15.30 1.000 15.30 1.000 15.30 1.000 15.30 1.000 15.30 1.000 15.30 1.000 1.000 15.30 1.000
ANISOU 1891 N VAL 27	5 1646 185	7 2417 -182 461 261
		





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ATOM 1953 CG PHE 283 14.842 3.269 41.512 1.000 14.75 ANISOU 1953 CG PHE 283 1985 1363 2255 12 -317 - 3 ANISOU 1954 CDI PHE 283 13.814 4.904 42.142 1.0000 21.50 ATOM 1954 CDI PHE 283 13.814 4.904 42.142 1.0000 21.50 ANISOU 1955 CD2 PHE 283 15.994 3.999 41.298 1.000 17.72 ATOM 1955 CD2 PHE 283 15.994 3.999 41.298 1.000 17.72 ANISOU 1955 CD2 PHE 283 15.994 3.999 41.298 1.000 17.72 ANISOU 1955 CD2 PHE 283 13.909 5.177 42.655 1.000 20.78 ATOM 1956 CE1 PHE 283 2056 1802 4036 92.66 -647 ANISOU 1957 CE2 PHE 283 2101 1257 2364 -5 -255 377 ANISOU 1957 CE2 PHE 283 16.115 5.290 41.814 1.000 15.06 ATOM 1957 CE2 PHE 283 16.115 5.290 41.814 1.000 15.06 ATOM 1958 CZ PHE 283 1881 1995 2979 192 -4322 0 ANISOU 1958 CZ ATOM 1959 N ASP 284 13.883 -1.178 42.579 1.000 13.07 ANISOU 1959 N ASP 284 13.883 -1.178 42.579 1.000 13.07 ANISOU 1959 CA ASP 284 141.502 -2.584 ATOM 1960 CA ASP 284 141.502 -2.584 ATOM 1961 C ASP 284 1407 ANISOU 1966 CD ASP 284 1407 ANISOU 1966 CD ASP 284 1407 ANISOU 1963 CB ASP 284 11.231 -3.147 ANISOU 1966 CD ASP 284 11.031 -3.147 ANISOU 1966 OD2 ASP 284 110.231 -3.147 ANISOU 1966 OD2 ASP 284 110.231 -3.147 ANISOU 1966 OD2 ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 OD2 ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1966 OD2 ASP 284 110.231 -3.147 ANISOU 1966 CD ASP 284 110.231 -3.147 ANISOU 1967 N VAL 285 112.04 -10.00 110.0	
ANISOU 1966 OD2 ASP 285 12.644 -2.191 40.217 1.000 12.40 ATOM 1967 N VAL 285 1582 1260 1870 79 -185 -131 ANISOU 1967 N VAL 285 1582 1260 39.216 1.000 12.31 ATOM 1968 CA VAL 285 11.599 -2.064 39.216 1.000 12.31 ANISOU 1968 CA VAL 285 1442 1469 1767 -161 -59 - 1 ANISOU 1969 C VAL 285 11.229 -3.419 38.589 1.000 12.09 ANISOU 1969 C VAL 285 1220 1407 1967 -1 -100 - 79 ANISOU 1970 O VAL 285 12.085 -4.311 38.433 1.000 13.68 ATOM 1971 CB VAL 285 1237 1514 2446 67 56 4 0 ANISOU 1971 CB VAL 285 12.009 -1.066 38.098 1.000 14.68 ATOM 1971 CB VAL 285 12.131 0.332 38.672 1.000 17.08 ATOM 1972 CG1 VAL 285 12.131 0.332 38.672 1.000 17.08 ANISOU 1972 CG1 VAL 285 2429 1402 2658 18 -465 425 ANISOU 1973 CG2 VAL 285 13.309 -1.499 37.433 1.000 15.69	
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ANISOU 1981 CA LEU 287 1812 1418 1631 ATOM 1982 C LEU 287 10.075 -3.654 32.908 1.000 15.12 ANISOU 1982 C LEU 287 1945 1714 2086 32 233 - 31 ANISOU 1983 O LEU 287 11.277 -3.883 32.927 1.000 17.91 ATOM 1983 O LEU 287 11.277 -3.883 32.927 1.000 17.91	

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ANTSON 1985 CG LEU 2		496 2523 .705 35.413	1.000 14.53
ATOM 1986 CDI LEU 2		444 2403	0 -146 143
ANIBOO IDOO ODD LETT 2		0.197 34.820	1.000 16.03
ATOM 1987 CD2 LEU 2	287 1476 2	035 2579	166 -100 - 7 1.000 15.09
ANISOU 1988 N ASP 2	288 9.256 -		73 175 - 216
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ATOM 1989 CA ASP 4	288 1992 2	2028 2268	29 335 - 314
ANISO0 1909 C ASP 2	288 10.437 -		1.000 18.74 -231 97 8 1
ANTSOU 1990 C ASP 2	288 2484 2	2597 2040 -2.526 29.849	1 000 25.48
ATOM 1991 O ASP 4		2422 3865	-322 639 340
ANISOU 1991 OF ACR	288 8.659	-5.490 30.060	1.000 19.23
ATOM 1992 CB ASP	288 2431	2414 2460	-209 258 -720 3 1.000 19.50
ATOM 1993 CG ASP	288 9.139	2499	-49 393 -554
ANTSON 1993 CG ASP	288 2688 288 10.173	2223 2499 -7.145 29.18	5 1.000 27.03
ATOM 1994 ODI ASP	288 3134	3038 4100	624 421 -110
ANIBOU ISSI TO TO	288 8.458	-6.566 27.95	5 1.000 31.00 307 -361 -2100
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ATOM 1996 N GLY	289 11.489 289 2960	2765	-531 7/8 IIO
ANISOU 1996 N GLY ATOM 1997 CA GLY	289 12.008	-3.083 28.16	9 1.000 25.60 -1469 558 1 1
ATOM 1997 CA GLY ANISOU 1997 CA GLY	289 3678	3562 2486	5 1 000 21.08
ATOM 1998 C GLY	289 12.988	2528	-485 353 1 3 0
ANISOU 1998 C GLY	289 2567 289 13.411	-2.097 29.89	1 1 . 0 0 0 2 3 . 7 2
ATOM 1999 O GLY ANISOU 1999 O GLY	289 3428	3219 2364	-1104 440 1 1 3 18 1.000 18.32
ATOM 2000 N GLU	290 13.402	2319	-145 616 -113
ANISOU 2000 N GLU	290 2246 290 14.538	-0.301 28.0	74 1.000 17.75
ATOM 2001 CA GLU ANISOU 2001 CA GLU	290 1912	2419 2412	97 770 - 30 1
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ANISOU 2002 C GLU	290 2180 290 15.143	2308 2313 1.619 29.3	53 1.000 17.58
ATOM 2003 O GLO		2050 2104	_35 380 103
ANISOU 2003 O GLU ATOM 2004 CB GLU	290 15.341	-0.161 26.7	85 1.000 23.21 -273 1753 -467
ANISOU 2004 CB GLU	290 3184	2508 3126 -1.492 26.2	26 1 000 24 . 55
ATOM 2005 CG GLU		222	348 1232 - / 4 3
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ANTSOU 2006 CD GLU	290 3365	3708 433	7 7 1 000 40.04
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ATOM 2008 OE2 GLU ANISOU 2008 OE2 GLU	J 290 8785	3812 707	406 1 000 18.14
ATOM 2009 N THE	R 291 13.004	210	3 224 /11 -24
ANISOU 2009 N THE		7 2.896 29.	049 1.000 18.72
ATOM 2010 CA THE ANISOU 2010 CA THE	R 291 2521	2080 251	1 105 1131 6 6 593 1.000 15.79
ATOM 2011 C THE	R 291 11.27	1750 206	(A 134 538 - 2 C
ANISOU 2011 C THI			217 1.000 18.62
ATOM 2012 O THE ANISOU 2012 O THE	R 291 2764	1966 234	14 -248 664 -311 .044 1.000 21.54
ATOM 2013 CB TH	IR 291 12.72		16 -164 891 362
ANISOU 2013 CB TH	IR 291 3043	2625 253	 ∪



- 80 --300 4 7 2430 -59 1509 ANISOU 2044 CG GLN 295 1391 33.115 1.000 13.56 295 0.157 6.687 2045 CD GLN-117 1 6 5 133 2361 1486 295 1305 ANISOU 2045 CD GLN 32.419 1.000 15.35 295 0.459 7.693 2046 OE1 GLN 161 206 220 2371 1651 295 1811 ANISOU 2046 OE1 GLN 32.943 1.000 15.04 295 -0.982 5.026 295 1225 1995 296 4.363 4.463 296 1425 1396 2047 NE2 GLN 2493 75 -139 - 99 MOTA ANISOU 2047 NE2 GLN 34.423 1.000 12.66 ASP 1990 181 -112 -110 2048 N MOTA 296 4.653 3.016 34.439 1.000 12.26 296 1628 1274 1755 53 -51 -151 ASP ANISOU 2048 N 2049 CA ASP MOTA ANISOU 2049 CA ASP 296 5.167 2.569 35.792 1.000 11.57 296 5.16/ 296 1199 1300 1.460 1895 -82 2050 C ASP 30 - 22 ATOM ANISOU 2050 C ASP 36.224 1.000 13.08 1.460 296 4.854 ASP 2070 -107 38 1 3 9 2051 0 296 1534 1368 ANISOU 2051 O ASP 33.399 1.000 14.18 2.634 296 5.709 2052 CB ASP 30 - 378 ATOM 1819 141 1700 296 1870 ANISOU 2052 CB ASP 2.84 1557 725 31.952 1.000 13.32 296 5.295 2053 CG ASP 67 2 1848 -58 ATOM 296 1655 ANISOU 2053 CG ASP 31.601 1.000 15.83 296 4.110 296 1680 2.725 2054 OD1 ASP -126 - 189 MOTA -68 2402 1935 ANISOU 2054 OD1 ASP 31.114 1.000 15.27 3.098 296 6.212 2055 OD2 ASP 2106 -229 137 177 MOTA 1937 296 1757 ANISOU 2055 OD2 ASP 36.416 1.000 12.26 297 6.038 3.352 1931 -34 -123 -118 TRP 2056 N ATOM1403 297 1325 ANISOU 2056 N TRP 37.656 1.000 12.82 297 6.683 2.960 2057 CA TRP -104 -49 151 MOTA 1599 1943 ANISOU 2057 CA TRP 297 1328 38.858 1.000 13.13 3.007 297 5.746 TRP \mathtt{ATOM} 2058 C 24 -23 1 8 5 1992 1580 297 1418 2.030 39.584 1.000 14.03 TRP ANISOU 2058 C 297 5.565 137 320 2059 0 TRP 1619 2159 102 MOTA 297 1554 ANISOU 2059 O 37.928 1.000 13.68 TRP 3.847 1692 297 7.908 TRP 2376 -19 -169 1 5 1 2060 CB MOTAANISOU 2060 CB TRP 297 1130 297 8.646 3.455 39.166 1.000 13.28 2061 CG TRP 2255 91 -96 2 2 MOTA 297 1143 1646 297 8.932 2.179 39.622 1.000 15.58 ANISOU 2061 CG TRP -544 - 77 2062 CD1 TRP MOTA 275 297 1615 1689 297 9.144 4.353 2618 40.189 1.000 14.69 ANISOU 2062 CD1 TRP
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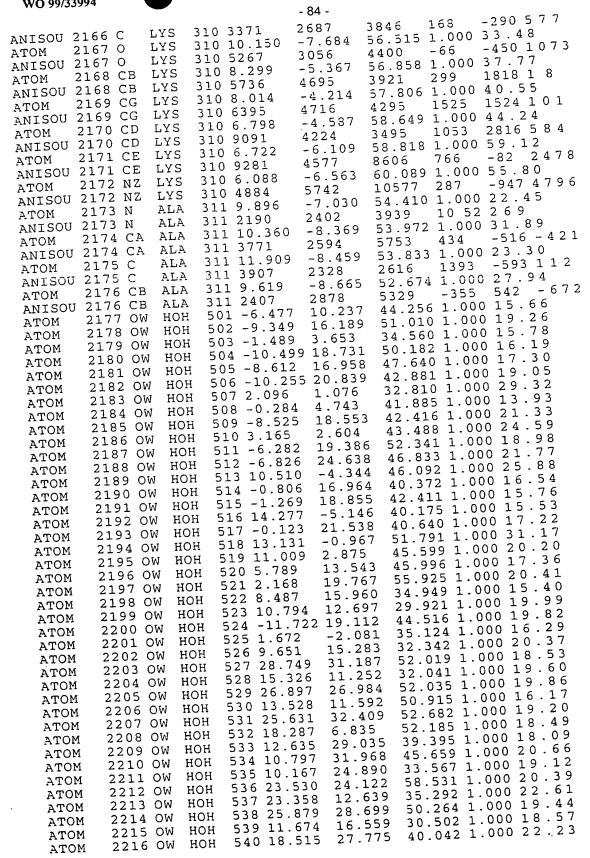
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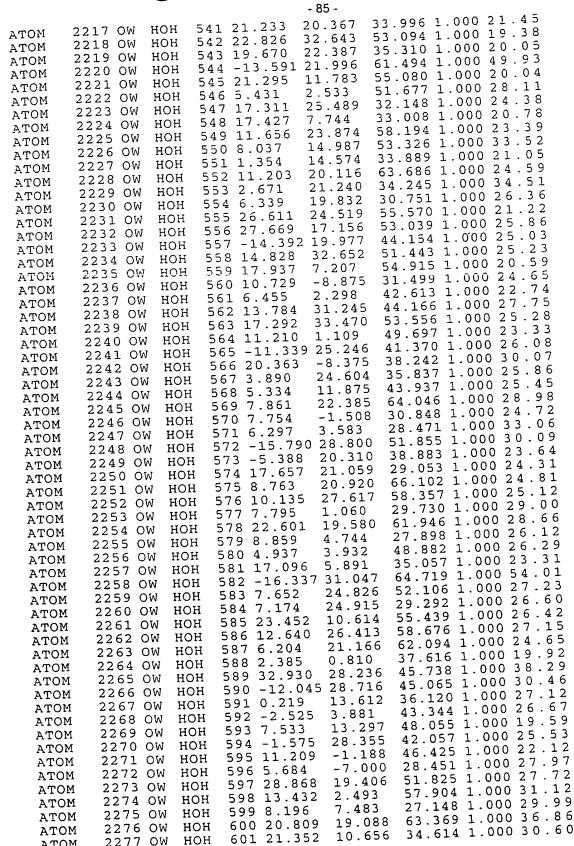
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ътОМ 2075 CG	1 ILE 298 5.907	6.245	41.001 1.000	-556 -1030
ATOM 2075 CO ANISOU 2075 CO	1 TLE 298 2776	4275	3525 -1314 41.929 1.000	25.05
ът∩м 2076 CC	32 TPE 730 3.012	6.319 3344	2405 -57	255 - 963
ANTSOU 2076 CO	32 ILE 298 3770		42.306 1.000	43.32
атом 2077 CI	O1 1LE 290 0.300	7224	1674 -652	-1890 -11/
ANTSOU 2077 CI	D1 ILE 298 4561 GLY 299 2.31		38 893 1.000	12.16
ATOM 2078 N			1879 78 -3	04 106
ANISOU 2078 N		8 3.741	38.670 1.000	12.98 -188 - 154
ATOM 2079 C ANISOU 2079 C	A GLY 299 1276	1279	2379 106	-189 - 134
ATOM 2080 C	GLY 299 0.13	5 5.017	38.378 1.000 2151 113	-231 1 1 8
ANISOU 2080 C	GLY 299 1421	1403 8 6.025		
атом 2081 О	GLY 299 0.73		2252 122	289 - 13
ANISOU 2081 O	GLY 299 1713 GLY 300 -1.1		38.447 1.000	13.08
ATOM 2082 N		-	2099 146	-267 -145
ANISOU 2082 N			37.992 1.000) 13.45 -415 - 143
ATOM 2083 C ANISOU 2083 C	· · · · · · · · · · · · · · · · · · ·	1521	2143 116	-415 - 1 4 5
	GLY 300 -2.5	19 6.972	39.042 1.000 2456 -52	-407 - 192
ATOM 2084 C ANISOU 2084 C	GLY 300 1098	3 1365	2456 -52 38.672 1.000	13.39
атом 2085 (GLY 300 - 3.4	262 7.875	2423 -19	-211 - 43
ANISOU 2085	O GLY 300 132	1342 973 6.845	40.254 1.00	0 13.35
атом 2086 1	N ASN 301 -1.		2151 -225	-232 - 104
ANISOU 2086			A1 313 1 00	0 13.83
ATOM 2087 ANISOU 2087		0 1435	2230 -194	-38 -61
ANISOU 2087 ATOM 2088	C ASN 301 -0.	837 8.254	41.885 1.00 1791 -35	-142 - 20
ANISOU 2088	C ASN 301 167	6 1268	42 169 1.00	0 13.89
атом 2089	O ASN 301 -0.	007 7.405 1 1355	2003 73 -	144 - 1 3
ANISOU 2089	O ASN 301 183 CB ASN 301 -3.		42 360 1.00	0 16.01
ATOM 2090			25/12 77 2	124 3 1 5
ANISOU 2090 ATOM 2091	-	942 8.199	43.106 1.00	152 - 90
ATOM 2091 ANISOU 2091	CG ASN 301 198	36 2508		
атом 2092	OD1 ASN 301 -4.	973 8.690	2204 -21	144 - 130
ANTSOU 2092	OD1 ASN 301 160)6 1626 518 8.454	44.338 1.0	00 33.30
ATOM 2093	ND2 ASN 301 -3 ND2 ASN 301 280		2028 101	2 -230 -1343
ANISOU 2093 ATOM 2094			42.073 1.0	00 12.96 -21 -135
ATOM 2094 ANISOU 2094		62 1278		00 13 48
atiom 2095	CA TYR 302 0.	674 9.948		0 -132 3 4
ANTSOU 2095	CA TYR 302 16	73 1259 768 9.269	0 74 078 1.0	00 12.63
ATOM 2096	C TYR 302 0.		2002 53	44 1 9
ANISOU 2096			1 44.806 1.0	100 14 . 15
ATOM 2097 ANISOU 2097		32 1737	2305 -65	48 - 27
ATOM 2098	R CB TYR 302 0.	764 11.4		33 4 1
ANTSOU 2098	3 CB TYR 302 16	35 1192		000 12.02
атом 2099	OCG TYR 302 L	159 12.1 86 1103	1000 -59	9 - 25 - 4/1
ANISOU 209	O CG TYR 302 15		33 41.275 1.	000 13.11
ATOM 210 ANISOU 210		633 1284	2066 -8	() 11 - 10
ATOM 210	1 CD2 TYR 302 0	.235 12.7		000 12.52 4 13 -127
ANTSOU 210	1 CD2 TYR 302 1	576 1132		000 12.29
ATOM 210	2 CE1 TYR 302 2	.933 12.8 581 1043	2 2045 -1	85 -84 - / /
ANISOU 210	2 CE1 TYR 302 1 3 CE2 TYR 302 0		273 39.535 1.	000 14.12
ATOM 210 ANISOU 210		462 144	3 2458 -2	41 15 3 4 5
ANISOU 210 ATOM 210	4 CZ TYR 302 1	.983 13.	347 39.241 1.	000 12.69 287 -91 1 0
ANISOU 210	4 CZ TYR 302 1	483 122	·	000 13.42
ATOM 210	5 OH TYR 302 2	2.376 13.	800 30.013 1	. = = =
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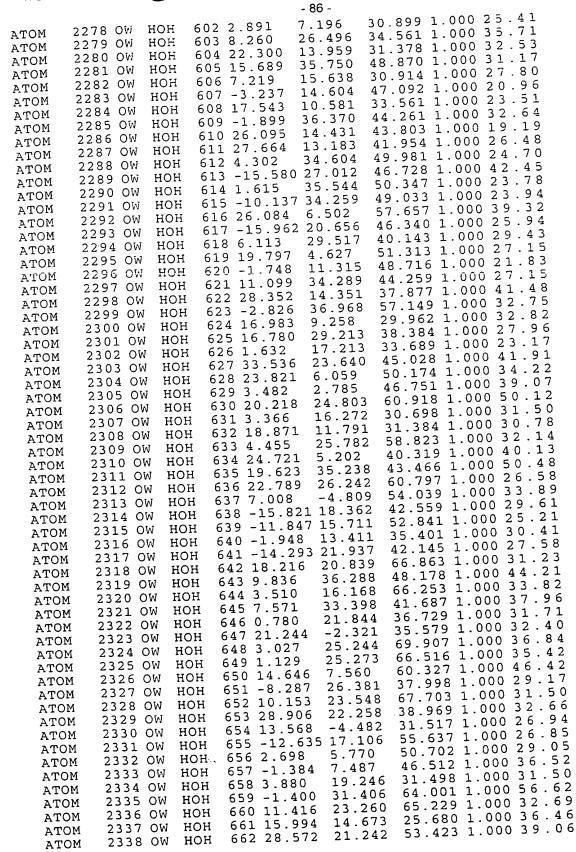
- 82 -33 1 4 6 -93 2124 1469 ANISOU 2105 OH TYR 302 1505 44.450 1.000 13.92 8.855 303 1.956 88 9 9 2106 N VAL 153 2246 1637 303 1406 45.746 1.000 14.51 VAL ANISOU 2106 N 8.336 303 2.355 2107 CA -391 - 74 VAL 2355 -137 ATOM 1320 303 1838 ANISOU 2107 CA VAL 46.239 1.000 15.23 9.244 303 3.498 -105 -348 VAL 2108 C -102 MOTA 2876 1507 303 1404 VAL 45.512 1.000 18.70 ANISOU 2108 C 9.386 303 4.471 VAL -239 326 -504 2109 0 MOTA 3386 303 1859 1861 VAL ANISOU 2109 0 45.632 1.000 16.75 6.880 303 2.856 16 - 759 - 123 2110 CB VALMOTA 2905 1319 303 2140 ANISOU 2110 CB 47.017 1.000 19.53 VAL303 3.279 6.401 2111 CG1 VAL 232 -1054 148 3284 1951 ANISOU 2111 CG1 VAL 303 2185 45.125 1.000 17.82 5.956 303 1.723 2112 CG2 VAL -213 -558 -406 MOTA 2852 1442 303 2476 ANISOU 2112 CG2 VAL 47.378 1.000 14.07 9.900 304 3.349 -39 -407 - 86 2113 N ASN MOTA 2566 1369 304 1409 10.928 47.772 1.000 14.31 ANISOU 2113 N ASN 304 4.317 2114 CA ASN -102 -424 - 55 MOTA 1387 2578 304 1474 304 5.450 ANISOU 2114 CA ASN 48.637 1.000 13.75 10.397 ASN 34 -274 - 87 2115 C MOTA 2378 1487 304 1360 ASN 48.584 1.000 14.60 ANISOU 2115 C 10.962 304 6.539 2116 0 ASN _55 *-*320 -34 MOTA 2438 1795 304 1314 48.551 1.000 14.26 ANISOU 2116 0 ASN12.035 304 3.589 6 -303 176 2117 CB ASN MOTA 2494 1214 304 1710 ANISOU 2117 CB ASN 47.642 1.000 14.81 304 2.535 12.661 2118 CG ASN 23 -114 402 MOTA 2449 1627 304 1551 ANISOU 2118 CG ASN 46.622 1.000 16.52 13.255 304 2.866 2119 OD1 ASN 80 19 5 8 9 MOTA 1746 2636 304 1896 12.595 48.102 1.000 18.43 ANISOU 2119 OD1 ASN 304 1.290 -10 199 2120 ND2 ASN 127 MOTA 2463 304 1560 2980 ANISOU 2120 ND2 ASN 49.463 1.000 16.36 9.413 305 5.175 -503 2 6 6 ILE 2121 N -78 MOTA 3117 1553 305 1546 50.407 1.000 14.85 ILE ANISOU 2121 N 8.890 305 6.173 165 -277 - 40 2122 CA ILE ATOM 2436 1537 305 1670 50.352 1.000 15.78 ANISOU 2122 CA ILE 7.372 305 6.183 95 -438 - 51 2123 C ILE ATOM 2914 305 1527 1555 49.886 1.000 17.54 ILE ANISOU 2123 C 6.736 305 5.231 3412 -131 -404 5 ILE 2124 0 MOTA 1789 305 1463 51.818 1.000 17.80 ANISOU 2124 O ILE 9.430 305 5.949 265 - 209 2125 CB ILE 2634 -23 MOTA 1962 305 2167 52.416 1.000 18.93 ANISOU 2125 CB ILE 9.091 305 4.578 1 -218 -163 2126 CG1 ILE MOTA 2526 305 1716 2948 10.944 51.823 1.000 19.17 ANISOU 2126 CG1 ILE 305 6.171 2127 CG2 ILE 70 -534 -405 MOTA 2737 305 2685 1863 53.863 1.000 21.28 ANISOU 2127 CG2 ILE 9.459 305 4.415 2128 CD1 ILE 19 452 - 71 MOTA 2662 2902 305 2521 50.908 1.000 14.59 ANISOU 2128 CD1 ILE 6.806 306 7.246 271 2129 N ARG 52 -356 MOTA 2165 1641 306 1738 50.828 1.000 15.25 ANISOU 2129 N ARG 5.360 306 7.424 2130 CA ARG -302 7 7 139 MOTA 2622 306 1509 1663 52.024 1.000 15.02 ANISOU 2130 CA ARG 4.903 306 8.234 -332 - 21 ARG 2131 C 133 MOTA 2656 1464 306 1588 52.433 1.000 16.63 ARG ANISOU 2131 C 5.614 -219 -294 -168 306 9.141 ARG 2132 0 MOTA 2536 2101 306 1682 49.532 1.000 16.31 ARG ANISOU 2132 O 4.943 306 8.135 -100 -270 -150 2133 CB ARG MOTA 2697 1681 306 1820 49.377 1.000 18.43 ARG ANISOU 2133 CB 3.414 306 8.226 40 -194 -156 2134 CG ARG MOTA 2828 1700 306 2476 47.900 1.000 18.26 ANISOU 2134 CG ARG 3.068 306 8.401 -120 -145 -330 ARG 2135 CD 2880 1971 306 2087 ANISOU 2135 CD ARG



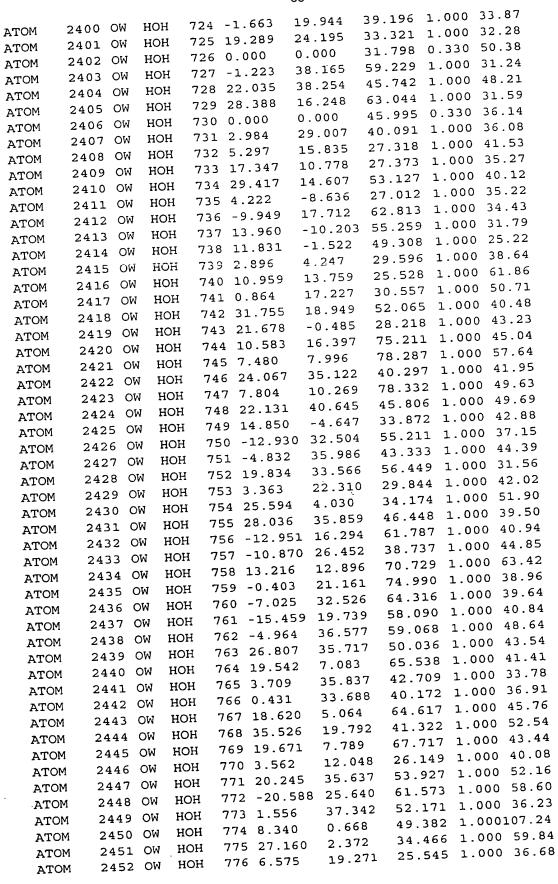


2277 OW

MOTA



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z mOM	2339 OW HOH	663 19.354 0.465	27.273 1.000 44.56
MOTA ATOM	2340 OW HOH	664 24.969 27.026	38.838 1.000 35.41 55.914 1.000 32.97
ATOM	2341 OW HOH	665 24.294 7.488	31.178 1.000 30.04
MOTA	2342 OW HOH	666 19.540 7.882 667 -9.236 32.988	57 241 1.000 39.20
MOTA	2343 OW HOH	667 -9.236 32.988 668 2.098 18.351	67 496 1.000 38.88
MOTA	2344 OW HOH 2345 OW HOH	669 11.390 3.245	56 270 1.000 37.56
ATOM	2345 OW HOH 2346 OW HOH	670 -21.413 24.449	52.026 1.000 44.66
ATOM ATOM	2347 OW HOH	671 -14.575 19.220	55.240 1.000 30.91
ATOM	2348 OW HOH	672 32.112 25.958	43.051 1.000 33.34 53.232 1.000 34.71
MOTA	2349 OW HOH	673 -15.050 31.151 674 2.941 -1.607	30.245 1.000 34.63
MOTA	2350 OW HOH	674 2.941 -1.607 675 26.951 14.544	34.757 1.000 49.17
MOTA	2351 OW HOH 2352 OW HOH	707 70 ((0)	39.386 1.000 30.55
ATOM	2352 OW HOH 2353 OW HOH	677 5.203 18.009	68 080 1.000 43 41
ATOM ATOM	2354 OW HOH	678 14.151 7.965	26.591 1.000 38.80
ATOM	2355 OW HOH	679 24.470 24.261	
ATOM	2356 OW HOH		
ATOM	2357 OW HOH	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	44 421 1.000 34.00
ATOM	2358 OW HOR 2359 OW HOR	202 2 202 2 255	45 456 1.000 35.39
ATOM	2359 OW HOF 2360 OW HOF	684 22.443 34.538	42.053 1.000 33.55
ATOM ATOM	2361 OW HOR	685 4 419 4 . 720	27.356 1.000 48.02 51.877 1.000 50.63
MOTA	2362 OW HO	i 686 -15.830 34.507	
ATOM	2363 OW HO		3 46 206 1.000 44.97
ATOM	2364 OW HOW 2365 OW HOW	1 212	29 272 1.000 35.15
MOTA	2365 OW HO! 2366 OW HO!	H 690 18.802 13.646	5 27.901 1.000 30.00
MOTA MOTA	2367 OW HO	н 691 6.997 17.523	29.313 1.000 47.70 7 69.105 1.000 36.97
ATOM	2368 OW HO		
MOTA	2369 OW HO	11 050 22 400 31 631	n 42 219 1.000 33.40
ATOM	2370 OW HO 2371 OW HO	11 051 001 00 00	2 30 744 1.000 34.21
${ t ATOM}$	2371 OW HO	н 696 6.897 22.41	
MOTA	2373 OW HO	Н 697 28.700 7.809	
ATOM	2374 OW HO		7 62 593 1.000 32.26
MOTA	2375 OW HC	17 01	0 43 200 1 000 43 20
MOTA	2376 OW HC 2377 OW HC	он 701 12.119 25.22	8 68.342 1.000 39.95
ATOM ATOM	2378 OW HO	NH 702 9.307 16.47	28.976 1.000 31.75 37 46.117 1.000 49.40
ATOM	2379 OW HO		
MOTA	2380 OW HO		36 802 1.000 38.55
ATOM		OH 705 24.764 7.530 OH 706 -22.095 25.66	59 59 047 1.000 36.71
ATOM ATOM		он 707 14.509 9.840	68.854 1.000 30.30
ATOM		OH 708 -10.129 28.72	42.036 1.000 38.92 10 48.390 1.000 35.29
ATOM	2385 OW H	OH 709 29.011 34.93	12 42 021 1.000 33.61
ATOM		2006 17 6	76 33 645 1.000 49.5/
ATOM	·	OH 711 -1.996 17.6 OH 712 10.216 17.7	48 26.015 1.000 41.04
ATOM ATOM		OH 713 23.535 29.6	
ATOM	1 2390 OW H	OH 714 20.488 -7.2	
ATOM	1 2391 OW H	OH 715 11.411 10.1	50 34 139 1.000 42.50
ATOM	· ·	OH 716 19.329 -4.2 OH 717 13.688 26.7	99 66 321 1.000 43.74
1OTA 1OTA		IOH 718 -10.751 33.0	064 54.747 1.000 40.47
ATOR		HOH 719 13.800 18.2	258 70.756 1.000 34.34
ATO	M 2396 OW H	HOH 720 17.151 5.81	36.691.0.330.27.42
ATO		1011	nn 41 559 0.330 37.77
ATO		HOH 722 0.000 0.00 HOH 723 15.314 7.54	
ATO!	M 2333 OW		



			-	89 -	
		77011 77	77 -17.605	29.205	62.661 1.000 56.83
MOTA	2453 OW	••	78 7.616	6.902	24.722 1.000 61.34
MOTA	2454 OW		79 19.749	10.700	68.006 1.000 65.22
MOTA	2455 OW	_	80 7.281	-5.270	50.090 1.000 50.00
MOTA	2456 W		81 -6.809	28.483	40.515 1.000 50.00
MOTA	2457 W		82 9.990	17.263	38.636 1.000 50.00
MOTA	2458 W	_		-2.331	28.939 1.000 50.00
ATOM	2459 W	_	83 5.767 84 11.694	-0.118	24.984 1.000 50.00
MOTA	2460 W			7.952	47.994 1.000 50.00
MOTA	2461 W	_	85 24.442 86 14.251	36.889	46.491 1.000 50.00
MOTA	2462 W			26.477	33.851 1.000 50.00
MOTA	2463 W			22.606	40.795 1.000 50.00
MOTA	2464 W			5.579	45.829 1.000 50.00
ATOM	2465 W				46.612 1.000 50.00
ATOM	2466 W			3.555	48.985 1.000 50.00
MOTA	2467 W	•••		13.464	28.121 1.000 50.00
MOTA	2468 W		792 9.397	10.442	42.781 1.000 50.00
MOTA	2469 W		793 28.257	17.944	59.241 1.000 50.00
MOTA	2470 W		794 4.652	15.287	79.554 1.000 50.00
MOTA	2471 W		795 5.977	11.852	47.616 1.000 50.00
MOTA	2472 W	_	796 30.501	14.258	54.367 1.000 50.00
MOTA	2473 W	-	797 5.625	20.228	33.277 1.000 50.00
MOTA	2474 W	HOH	798 23.942	14.642	58.997 1.000 50.00
MOTA	2475 W	HOH	799 10.164	31.943	52.999 1.000 50.00
MOTA	2476 W	HOH	800 7.807		34.817 1.000 50.00
MOTA	2477 W	HOH	801 23.377	_	32.004 1.000 50.00
MOTA	2478 W	HOH	802 21.193		1 000 E0 00
MOTA	2479 W	HOH	803 34.928		*** 50 00
MOTA	2480 W	HOH	804 29.073	-2.049	- 222 50 00
MOTA	2481 W		805 7.008		45.531 1.000 50.00
ATOM	2482 W	HOH	806 25.363		55.971 1.000 50.00
MOTA	2483 W	HOH	807 30.704		000 EO OO
MOTA	2484 W	HOH	808 33.072		000 50 00
ATOM	2485 W	HOH	809 -15.5		000 EO OO
MOTA	2486 W	HOH	810 6.072	18.137	7 25.000 EO OO
ATOM	2487 V	HOH	811 -7.21	4 39.940	
ATOM	2488 V	4 HOH	812 5.509	18.51	56.672 1.000 50.00
MOTA	2489 V	NOH	813 33.84		
MOTA		HOH W	814 0.421	35.77	
ATOM		HOH W	815 35.28		J 40.000 = 200 E0 00
ATOM		HOH W	816 39.34		3 40.0.2
ATOM		HOH W	817 -5.19		0 00.030 - 000 50 00
ATOM		M HOH	818 30.19		- 000 50 00
ATOM		HOH W	819 -4.86		4 01.752 = 1 000 E0 00
ATOM		и нон	820 -14.5		2 500 50 00
MOTA		м нон	821 1.340		
OTA		м нон	822 34.5		
OTA		W HOH	823 32.1		,1 32.2.
OTA		W HOH	824 13.5		200 50 00
ATO!			07	2 -4.1	41 27.534 1.000 50.00
AIO	. 2502				

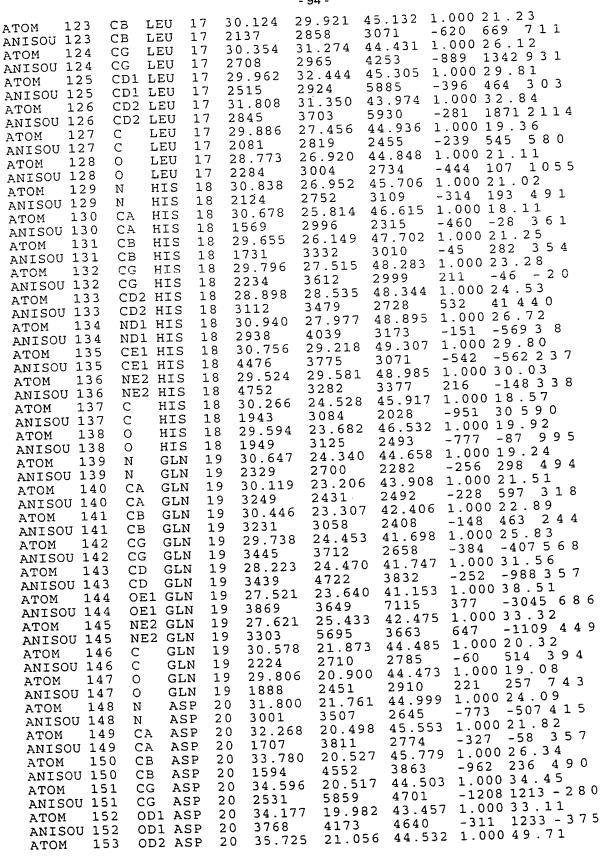
STRUCTURE B

STRUC	TURE B	
ATOM 1 ANISOU 1 ATOM 2 ANISOU 2 ATOM 3 ANISOU 3 ATOM 4 ANISOU 4 ATOM 5 ANISOU 5 ATOM 6 ANISOU 6 ATOM 7 ANISOU 7 ATOM 8 ANISOU 9 ATOM 10 ANISOU 10 ATOM 11 ANISOU 11 ATOM 12 ANISOU 12 ATOM 13 ANISOU 12 ATOM 13 ANISOU 14 ANISOU 15 ANISOU 15 ANISOU 15 ANISOU 15 ANISOU 16 ANISOU 16 ANISOU 17 ANISOU 18 ANISOU 19 ANISOU 20 ANISOU 21 ANISOU 21 ANISOU 22 ANISOU 22 ANISOU 23 ANISOU 24 ANISOU 25 ANISOU 26 ANISOU 27	TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT	28.901 15.176 58.379 658 -390 - 615 2232 4393 4489 60.597 1.000 29.41 28.467 15.029 60.597 1.000 29.41 27.046 14.764 60.421 1.000 28.55 27.046 14.764 60.421 1.000 36.51 26.447 13.762 61.414 1.000 36.51 26.447 13.762 62.758 1.000 42.45 26.629 14.220 62.758 1.000 42.45 27.153 12.412 61.315 1.000 50.26 27.153 12.412 61.315 1.000 50.26 27.153 12.412 61.315 1.000 29.01 26.240 16.061 60.553 1.000 29.01 25.041 16.044 60.827 1.000 35.82 25.041 16.044 60.827 1.000 35.82 25.041 16.044 60.332 1.000 24.98 26.928 17.181 60.332 1.000 24.98 26.928 17.181 60.332 1.000 24.98 26.214 18.465 60.327 1.000 23.97 24.26 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 344 -1563 -3.75 3437 2426 3244 39.500 26.40 3988 2812 6184 195 -2081 -1134 398 2812 6184 195 -2081 -1134 398 2812 6184 195 -2081 -1134 398 2812 6184 195 -2081 -1134
ANISOU 26 ATOM 27 ANISOU 27	CB THR OG1 THR OG1 THR	4 2636 2429 310351 1.000 32.62 4 28.050 19.484 61.551 1.000 32.62 4 3398 2812 6184 195 -2081 -1134 4 26.429 20.942 60.663 1.000 26.40 26.429 20.942 60.663 1.000 26.40
	G CG2 THR C THR C THR C THR C THR	4 2373 2692 4967 533 534 4 25.325 18.577 59.097 1.000 21.64 4 25.325 18.577 59.097 1.000 21.64 4 3090 2760 2374 368 -750 - 20 4 3090 15.88 4 25.738 18.264 57.980 1.000 21.58 4 2668 2629 2902 246 -560 - 659 4 2668 2629 2902 1.000 15.88
ATOM 3		5 24.104 19.049 59.340 1.000 13.80

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		- 91 -	1508 -613 -630 - 162
ANISOU 31	., ,,,,,	305 2021 3.211 19.385	58.211 1.000 14.80
ATOM 32 ANISOU 32	CA VAL 5 24	163 1893	1266 -594 -473 - 87
ATOM 33	CB VAL 5 21	1.742 19.402	58.606 1.000 16.09 1757 -412 -406 5 0 2
ANISOU 33	CD 1-1-	476 1881 0.855 19.846	57 447 1.000 14.91
ATOM 34		468 1859	1337 9 -102 197
ANISOU 34 ATOM 35	CG2 VAL 5 2:	1.310 17.994	59.074 1.000 21.15 2677 -700 -418 1198
ANISOU 35	CG2 VAL 5	015 2345 3.639 20.762	57 694 1.000 17.70
атом 36		893 2085	1749 -1137 -713 1 0 3
ANISOU 36 ATOM 37	O VAL 5 2	3.532 21.759	58.419 1.000 17.35 2050 -698 -650 1 0 5
ANISOU 37	0 VAL 5 2	566 1978 4.150 20.845	2050 -698 -650 1 0 5 56.479 1.000 13.23
ATOM 38	.,	4.150 20.845 334 1597	2097 -162 -658 4 0 9
ANISOU 38 ATOM 39	CD PRO 6 2	4.302 19.770	55.484 1.000 15.56 2176 -309 -383 2 7 7
ANISOU 39	CD PRO 6 1	.887 1850	2176 -309 -383 2 7 7 56.005 1.000 14.49
ATOM 40	· · · · · · · · · · · · · · · · · · ·	24.667 22.137 332 1740	2432 -218 -536 5 2 2
ANISOU 40 ATOM 41	CA PRO 6 1 CB PRO 6 2	25.571 21.722	54.847 1.000 18.21
ANISOU 41	CB PRO 6	2294 1740	2000
ATOM 42		25.132 20.378 2708 2632	2399 -1078 38 - 61
ANISOU 42		23.576 23.091	55.510 1.000 14.59
ATOM 43 ANISOU 43	C PRO 6	1388 1712	2123
ATOM 44		22.408 22.743 1298 1547	2118 -283 -596 1 5
ANISOU 44 ATOM 45		24.048 24.326	5 55.313 1.000 14.56
ATOM 45 ANISOU 45	N THR 7	1393 1678	2400 - 1 000 10 00
ATOM 46	C11	23.288 25.428 1463 1584	1998 -469 -734 4 4 0
ANISOU 46 ATOM 47		23.121 26.572	2 55.799 1.000 14.44
ANISOU 47	CB THR 7	1927 1652 22.454 26.10	2 56 998 1,000 18 44
ATOM 48	OG1 THR 7 OG1 THR 7	22.454 26.103 3136 2013	1858 -333 -829 1 7 6
ANISOU 48 ATOM 49	CG2 THR 7	22.290 27.71	9 55.261 1.000 14.98 2513 -213 -727 4 1 2
ANISOU 49	CG2 THR 7	1390 1788 23.973 26.00	E 53 539 1 000 14.62
ATOM 50	C THR 7 C THR 7	23.973 26.00 1144 2200	2212 -355 -693 7 0 4
ANISOU 50 ATOM 51	O THR 7	25.192 26.25	7 53.600 1.000 17.21 2738 -641 -840 9 7 5
ANISOU 51	O THR 7	1284 2515 23.211 26.22	12 52 472 1 000 12.32
ATOM 52		1165 1596	1919 -314 -534 3 7 0
ANISOU 52 ATOM 53		23.692 26.86	59 51.283 1.000 13.31 1971 -60 -295 3 4 3
ANISOU 53		1554 1531 23.724 25.93	33 50.067 1.000 13.71
ATOM 54 ANISOU 54		1479 1705	2025 -136 -232 234
ATOM 55	CG PHE 8	24.635 24.74 1225 1716	46 50.258 1.000 13.68 2257 -185 8 155
ANISOU 55		1225 1716 24.147 23.5	03 50.628 1.000 14.10
ATOM 56 ANISOU 56		1317 1710	2329 - 93 231 221
ATOM 5	7 CD2 PHE 8	26.006 24.8 1239 2282	$\frac{1}{3134}$ -234 -56 91
ANISOU 57	7 CD2 PHE 8 8 CE1 PHE 8	1239 2282 24.984 22.4	20 50.812 1.000 15.39
ATOM 53 ANISOU 5	8 CE1 PHE 8	1473 1878	233
ATOM 5	9 CE2 PHE 8	26.840 23.8 1179 2259	3301 -157 -143 4 2 3
ANISOU 5 ATOM 6	9 CE2 PHE 8 0 CZ PHE 8	26.348 22.5	67 50.654 1.000 17.12
ANISOU 6	O CZ PHE 8	1310 2437	73 50 909 1.000 12.76
ATOM 6	1 C PHE 8	22.821 28.0 1401 1513	3, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
ANISOU 6	1 C PHE 8	T407 T07	

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ANISOU 8 ATOM 8 ANISOU 8 ATOM 8 ANISOU 8 ATOM 9 ANISOU 9 ANISOU 9 ATOM 9	O PHE 8 1392 1295 2322 2-56 -400 3 6 4 N SER 9 1392 1295 2322 -256 -400 3 6 4 N SER 9 1722 1636 1593 -565 -601 49 0 SER 9 1722 1636 1593 -565 -601 49 0 SER 9 1722 1636 1593 -565 -601 49 0 SER 9 1591 1468 1708 -392 -438 3 1 5 CA SER 9 1591 1468 1708 -392 -438 3 1 5 CA SER 9 23.743 31.472 49.761 1.000 15.41 SER 9 23.138 32.539 49.007 1.000 17.99 3 GG SER 9 23.138 32.539 49.007 1.000 17.99 9 2 4 CA SER 9 22.520 29.868 48.276 1.000 12.72 CA SER 9 22.520 29.868 48.276 1.000 12.72 CA SER 9 22.520 29.868 48.276 1.000 12.72 CA SER 9 23.397 29.495 47.478 1.000 16.18 SER 9 22.520 29.868 48.276 1.000 14.19 N LEU 10 2154 1488 1750 -301 -699 17 4 SER 9 10 SER 9 22.520 1880 -465 -3817 3 SER 9 10 SER 9 22.520 1880 -465 -3817 3 SER 9 22.52 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.52 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.52 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.5 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.5 SER 9 20.50 1800 -465 -3817 3 SER 9 22.5 SER 9 20.40 1187 1606 -411 -576 4 7 6 SER 9 20.5 SER 9 20.00 14.10 10 2154 1488 1750 -301 -699 17 4 SER 9 SER 9 20.5

- 93 --140 -170 4 9 8 1713 1873 1734 27.248 44.620 1.000 15.37 LEU 13 C.A. ANISOU 92 24.003 LEU 13 CB-375 -149 4 6 5 93 1838 1795 2205 13 ANISOU 93 CB LEU 1.000 14.52 26.554 45.967 24.154 13 LEU -280 -204 4 4 2 CG 1799 1803 1913 LEU 13 ANISOU 94 CG 1.000 15.15 46.193 25.680 22.934 CD1 LEU -433 185 175 95 MOTA 1766 1817 2174 CD1 LEU 13 46.067 1.000 17.54 ANISOU 95 25.690 25.411 CD2 LEU 13 -419 2 7 0 MOTA 96 -38 2502 2043 2119 13 CD2 LEU ANISOU 96 42.725 1.000 16.54 28.626 24.876 13 LEU 97 C -222 -93 565 MOTA 1710 2062 LEU 13 2510 ANISOU 97 С 41.821 1.000 18.28 28.122 25.548 LEU 13 0 -687 75 2 5 9 98 ATOM 1748 2514 2685 LEU 13 29.534 42.472 1.000 16.86 ANISOU 98 0 23.945 GLN 14 N 99 -557 -683 8 3 8 ATOM 2337 2100 1970 1423.657 30.015 41.132 1.000 18.63 ANISOU 99 GLNN 14 CAGLN-610 -802 5 6 8 100 ATOM 1915 2404 2761 14 GLN 30.923 41.130 1.000 19.39 ANISOU 100 CA22.421 14 GLN -392 -918 9 7 7 101 CB ATOM 2025 3166 2176 14 CВ GLN 30.250 41.460 1.000 19.00 ANISOU 101 21.108 14 GLN -209 -725 4 6 0 102 CG MOTA 1957 2383 2879 14 31.227 41.766 1.000 18.83 GLN CG ANISOU 102 19.974 14 GLNCD-6 -1229 4 9 4 103 MOTA 1897 2118 3139 14 GLN 32.317 42.314 1.000 26.10 ANISOU 103 CD 20.177 OE1 GLN 14 -1172 -241 ATOM 104 -98 2407 3582 3928 14 18.745 30.823 41.411 1.000 20.94 OE1 GLN ANISOU 104 NE2 GLN 14 -149 -840 4 5 4 105 ATOM 2340 2716 2900 24.804 30.812 40.525 1.000 20.40 14 ANISOU 105 NE2 GLN 14 -795 -712 9 3 7 GLN 106 С MOTA 2065 2458 3226 14 30.951 39.311 1.000 30.48 ANISOU 106 ${\tt GLN}$ С 24.812 -2337 -898 1211 ${\tt GLN}$ 14 107 0 MOTA 2152 5089 4340 14ANISOU 107 GLN41.329 1.000 20.35 0 31.309 25.734 GLN 15 -1067 -240 4 9 7 N 108 ATOM 2030 3252 2452 15 32.041 40.884 1.000 21.88 ANISOU 108 N GLN 26.909 15 GLN-1152 -299 7 8 8 109 CA ATOM 1901 3230 15 3184 GLN27.288 33.100 41.920 1.000 22.20 ANISOU 109 CA-1131 -770 6 9 1 GLN15 CB 110 MOTA 2551 3162 26.450 34.358 41.954 1.000 25.73 2720 15 GLNANISOU 110 CB 15 -821 -233 1 2 6 9 GLN CG 111 ATOM 2735 2545 15 4496 35.021 43.306 1.000 35.76 GLNANISOU 111 CG 15 26.325 -643 -229 -135 GLN CD 112 MOTA 3631 3945 15 6010 34.884 44.225 1.000 49.13 GLN ANISOU 112 CD 27.145 15 -2857 -2197 -564 OE1 GLN 113 MOTA 4378 5866 8425 15 OE1 GLN 43.489 1.000 51.85 ANISOU 113 35.812 25.255 15 NE2 GLN 62 3066 107 114 MOTA 5567 6945 7190 NE2 GLN 15 40.625 1.000 23.93 ANISOU 114 31.079 28.069 15 115 GLN -990 145 884 С MOTA 2127 3513 15 3451 31.448 40.213 1.000 28.95 GLNANISOU 115 29.177 ${\tt GLN}$ 15 -899 510 1225 116 0 MOTA 2845 4619 3535 29.794 40.891 1.000 25.86 GLN 15 ANISOU 116 0 27.828 GLY 16 -889 -36 469 117 N MOTA 2457 3282 4089 16 40.649 1.000 29.00 GLY ANISOU 117 N 28.763 28.812 GLY 16 -677 765 255 CA118 MOTA 2671 3562 4785 16 28.546 41.814 1.000 25.45 ANISOU 118 CAGLY GLY 29.741 16 -264 1422 673 С 119 MOTA 2754 3490 3427 GLY 16 С 41.625 1.000 29.63 ANISOU 119 30.805 27.955 GLY 16 1997 5 2 3 Ω 120 MOTA -66 4068 3267 3925 16 GLY ANISOU 120 0 43.015 1.000 22.50 28.979 29.387 17 923 733 LEU Ν MOTA 121 -39 2569 2713 3266 17 ANISOU 121 LEU 44.172 1.000 21.73 N 28.727 30.234 17 LEU -282 867 748 CA MOTA 122 3025 2931 17 2299 LEU ANISOU 122 CA

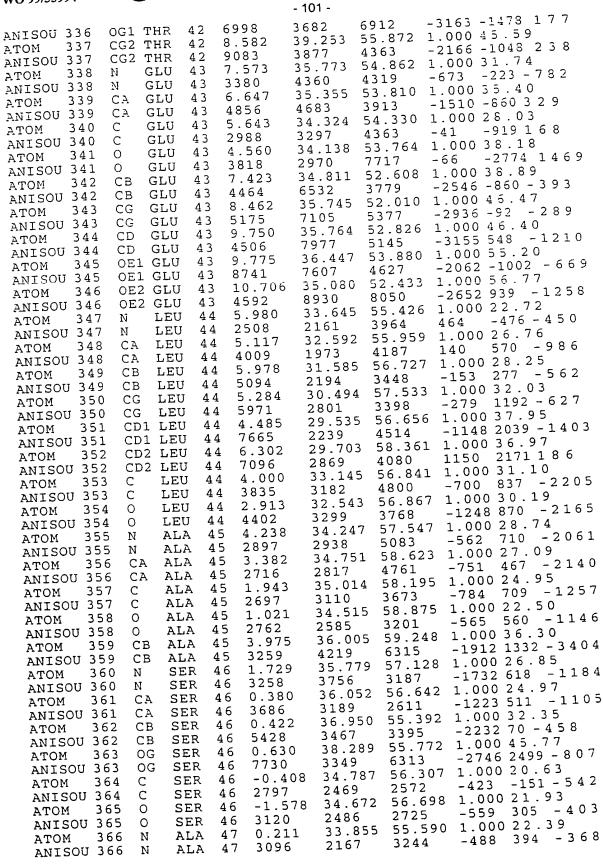


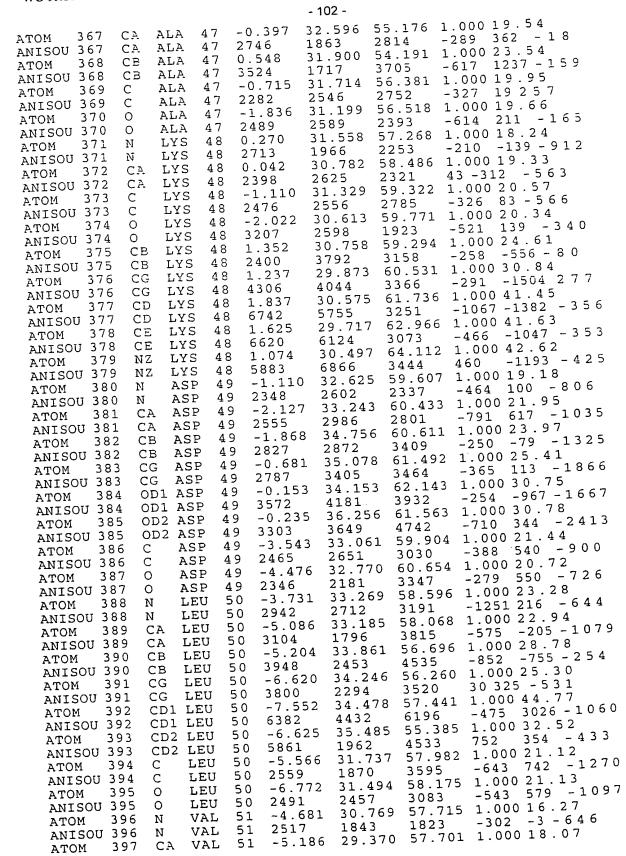
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ATOM 184 NH2 ARG 23 31 830 20.114 41.340 1.000 36.08 ANISOU 184 NH2 ARG 23 2261 5328 6121 -562 776 -86 ATOM 185 C ARG 23 2261 5289 167 -32 -23 4 ANISOU 185 C ARG 23 21071 2061 2589 167 -32 -23 4 ANISOU 186 O ARG 23 27.335 15.687 46.410 1.000 16.28 ATOM 185 O ARG 23 27.335 15.687 46.410 1.000 16.28 ANISOU 186 O ARG 23 27.335 15.687 46.410 1.000 16.28 ANISOU 187 N ARG 24 20.94 2156 2623 -52 -21 29 ANISOU 187 N ARG 24 20.94 2156 2623 -52 -21 29 ANISOU 188 CA ARG 24 1443 2589 2693 275 -22 15 ATOM 187 N ARG 24 1443 2589 2693 275 -22 15 ATOM 187 N ARG 24 1443 2589 2693 275 -22 15 ATOM 188 CA ARG 24 1443 2589 2693 275 -22 15 ATOM 188 CA ARG 24 1443 2589 2693 275 -22 15 ATOM 189 CB ARG 24 1443 2589 2693 275 -22 15 ATOM 189 CB ARG 24 1443 886 3289 484 -2573 84 ANISOU 189 CB ARG 24 1443 886 3289 484 -2573 84 ANISOU 190 CG ARG 24 1443 85078 5057 426 441 30 8 ANISOU 191 CD ARG 24 1163 5831 5736 208 370 45 8 ATOM 191 CD ARG 24 1163 5831 5736 208 370 45 8 ATOM 192 CD ARG 24 1163 5831 5736 208 370 45 8 ATOM 192 CD ARG 24 178 30 8 ANISOU 191 CD ARG 24 4738 6888 6124 -1719 -1822 13 16 ANISOU 193 CD ARG 24 33.973 18.776 49.903 1.0004 4.24 ATOM 194 NIH ARG 24 33.793 18.776 49.903 1.0004 4.24 ATOM 194 NIH ARG 24 33.793 18.776 49.903 1.0004 4.24 ATOM 195 NIH2 ARG 24 5339 4428 6503 513 -991 1216 ATOM 197 O ARG 24 1706 1890 2247 79.384 1.000 17.16 67 ATOM 197 O ARG 24 1706 1890 2247 79.384 1.000 17.16 67 ATOM 198 N CYS 25 907 1824 2176 -254 -386 1.51 ATOM 199 CR 275 25 5600 18.497 19.871 1.000 11.50 ATOM 200 CC CYS 25 893 1897 1645 -278 384 1.000 17.16 67 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.16 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.00 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.00 ATOM 200 CC CYS 25 5001 16.225 49.769 1.000 11.7.00 ATOM 200 CC CYS 25
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ANISOU 219 NH ATOM 220 NH ANISOU 221 C ANISOU 221 C ATOM 222 O ANISOU 222 O ANISOU 223 N ANISOU 223 N ANISOU 224 CA ANISOU 224 CA ANISOU 225 CA ANISOU 225 CA ANISOU 225 CA ANISOU 226 CA ANISOU 226 CA ANISOU 227 ANISOU 227 ANISOU 227 ANISOU 227 ANISOU 228 ANISOU 228 ANISOU 228 ANISOU 229 ANISOU 229 ANISOU 230 ANISOU 231 ANISOU 231 ANISOU 231 ANISOU 231 ANISOU 231 ANISOU 231 ANISOU 232 ANISOU 233 ANISOU 233 ANISOU 233 ANISOU 234 ANISOU 235 ANISOU 235 ANISOU 235 ANISOU 236 ANISOU 237 ANISOU 237 ANISOU 238 ANISOU 238 ANISOU 238 ANISOU 238 ANISOU 238 ANISOU 239	A SP 28 ASP 28 A	2259 2356 1861 517 49 - 248 27.502 10.780 46.801 1.000 25.08 3110 2837 3583 1105 606 - 399 28.995 10.992 46.457 1.000 30.32 2976 3836 4710 1190 720 - 1381 29.818 11.407 47.581 1.000 36.51 3633 4937 5301 121 391 - 1429 30.988 12.019 47.560 1.000 38.07 3334 5192 5941 364 661 - 1776 31.565 12.340 46.401 1.000 48.56 4482 7688 6280 -1305 736 - 1326 31.606 12.328 48.701 1.000 40.23 2891 6127 6266 457 717 - 2463 324.968 10.499 49.072 1.000 14.66 1720 1617 2233 135 - 33 - 42 24.968 10.499 49.973 1.000 15.33 314 98	4 5 5 3
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ANISOU 261 ATOM 262 ANISOU 263 ANISOU 263 ANISOU 264 ANISOU 264 ANISOU 265 ANISOU 265 ANISOU 266 ANISOU 266 ANISOU 267 ANISOU 267 ANISOU 268 ATOM 268 ANISOU 268 ATOM 268 ANISOU 268 ATOM 270 ANISOU 2	O PHE N TYR N TYR N TYR CA TYR CA TYR CB TYR CB TYR CB TYR CG TYR CG TYR CD1 TYR CD1 TYR CD2 TYR CD3 CC2 TYR CC2 TYR CC3 CC4 TYR CC4 CC7 TYR C	32 1015 1042 1042 1042 1042 1000 11.29 1286 1906 -95 -495 -7 -7 -7 -33 19.736 23.099 54.493 1.000 12.68 19.736 23.099 54.493 1.000 10.64 10.64 10.53 2158 -57 -766 -15 133 18.945 24.335 54.607 1.000 10.64 10.64 10.000 10.64 10.000 10.85 10.000 10.000 11.000 11.000 11.000 11.000 11.000 11.0000 11.000 11.000 11.000 <th>5 9 3 2 6 4 1 7 6 2 7 3 3 0 0 4 9</th>	5 9 3 2 6 4 1 7 6 2 7 3 3 0 0 4 9





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ANISOU 401 C VAL 51 3154 1763 1947 -401 -15 -427 ANISOU 398 CB VAL 51 -4.281 28.415 56.889 1.000 16.07 ANISOU 399 CG1 VAL 51 2981 1629 1496 -621 -255 -50 1 ANISOU 399 CG1 VAL 51 2981 1629 1496 -621 -255 -50 1 ANISOU 399 CG1 VAL 51 2981 1629 1496 -621 -255 -50 1 ANISOU 400 CG2 VAL 51 2959 2382 1875 -383 -100 3 0 2 ANISOU 400 CG2 VAL 51 4569 2121 1728 -1393 64 -86 9 ANISOU 401 C VAL 51 -5.446 28.899 59.114 1.000 17.74 ANISOU 401 C VAL 51 -6.430 28.187 59.346 1.000 19.76 ANISOU 402 O VAL 51 -6.430 28.187 59.346 1.000 19.76 ANISOU 403 N ILE 52 2980 2945 1760 -649 364 -9 0.2 ATOM 404 CA ILE 52 2980 2945 1760 -649 364 -9 0.2 ATOM 404 CA ILE 52 2980 2945 1760 -649 364 -9 0.2 ANISOU 405 CB ILE 52 -3.847 29.230 62.469 1.000 20.17 ANISOU 406 CG2 ILE 52 3294 3151 1652 -449 462 -1043 ANISOU 406 CG2 ILE 52 3294 3151 1652 -449 462 -1043 ANISOU 407 CG1 ILE 52 -2.619 28.346 62.217 1.000 20.23 ATOM 408 CG1 ILE 52 -2.619 28.346 62.217 1.000 20.25.37 ANISOU 408 CD1 ILE 52 3213 3819 2608 -307 727 -109 0 ANISOU 409 C ILE 52 3474 29.514 61.950 1.000 22.3.23 ATOM 409 C CILE 52 3474 29.514 61.950 1.000 22.3.23 ATOM 409 C ILE 52 3474 29.514 61.950 1.000 23.23 ATOM 409 C ILE 52 3474 29.514 61.950 1.000 23.23 ATOM 409 C ILE 52 3119 3216 62.470 1.000 23.23 ATOM 409 C ILE 52 3390 3654 1719 -362 529 -68 9 ANISOU 409 C ILE 52 3474 29.514 61.950 1.000 23.23 ATOM 410 0 ILE 52 3390 3654 178 1 100 22.44 ANISOU 408 CD1 ILE 52 3390 3664 62.217 1.000 23.23 ATOM 410 N ASP 53 -6.519 30.754 61.597 1.000 23.23 ATOM 411 N ASP 53 2897 3064 2903 -6266 700 -1361 ANISOU 411 N ASP 53 2897 3064 2903 -6266 700 -1361 ANISOU 412 CA ASP 53 -7.942 3335 4235 -4238 419 -1446 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4238 70 -1446 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4238 70 -1446 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4238 70 -1446 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4235 -4238 3349 61.570 1.000 27.43 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4235 -4234 4146 ANISOU 413 CB ASP 53 -7.942 33335 4235 -4235 -4234 4235 -4234 4235 -4234 42
ATOM 415 OD1 ASP 53



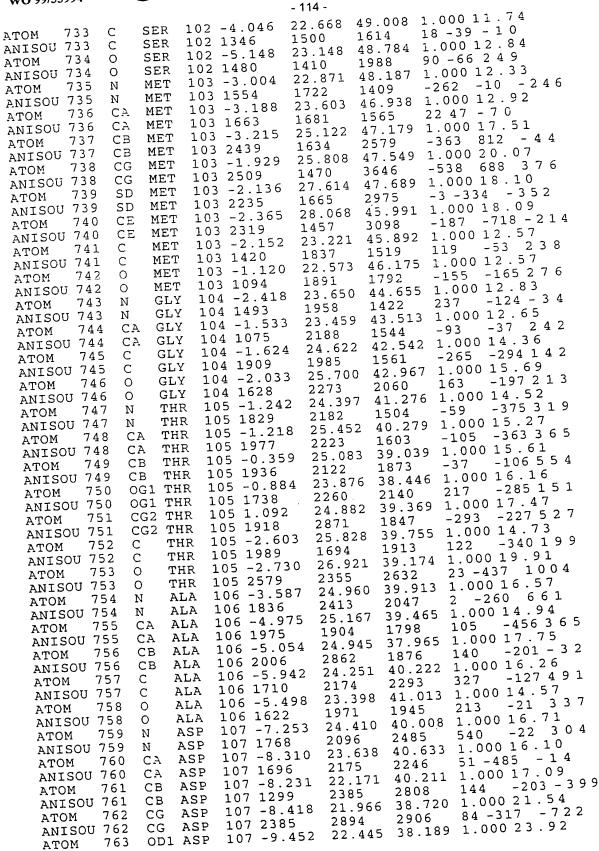
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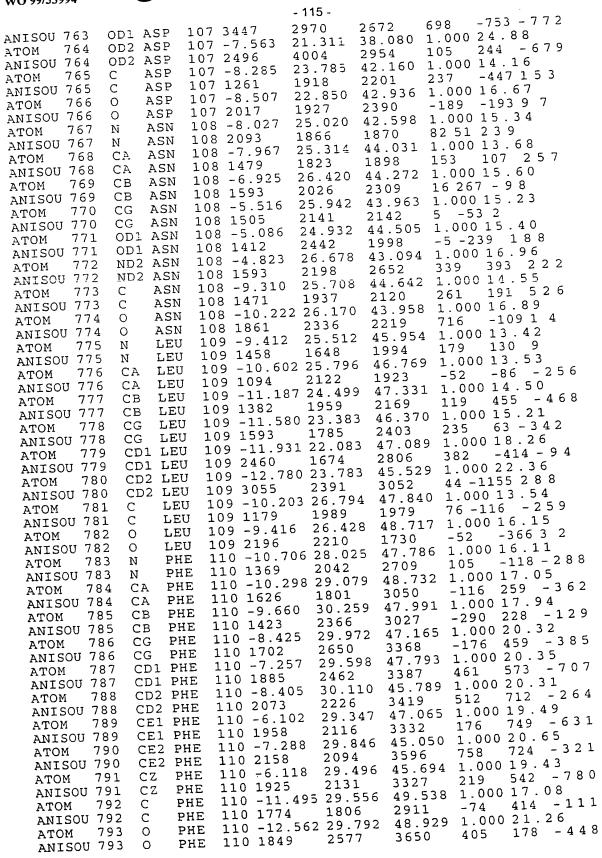
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- 112 -16.975 62.750 1.000 22.54 -9.924 95 SER CA 672 -120 -301 4 6 MOTA 2603 3706 95 2257 SER CA64.163 1.000 23.58 ANISOU 672 17.106 95 -9.370 С SER -521 -88 -85 673 ATOM 3671 3478 SER 1811 95 ANISOU 673 18.034 64.481 1.000 26.53 -8.623 95 SER -469 -167 -641 MOTA 674 0 4247 3242 2592 SER 95 -10.838 18.177 62.478 1.000 27.58 ANISOU 674 0 95 SER CВ 675 ATOM -379 2 8 4264 365 2556 3657 95 -11.506 18.093 61.242 1.000 39.40 SER CB ANISOU 675 95 676 OG SER -1445 1442 ATOM 900 4421 4214 95 6336 ANISOU 676 SER -9.712 16.194 65.060 1.000 25.04 OG 96 ASP 677 N -399 277 -232 MOTA 3248 3688 2579 96 ASP -9.228 16.317 66.422 1.000 24.42 ANISOU 677 Ν 96 ASP -470 257 -526 CA678 ATOM 3347 3330 2603 96 ASP -7.735 16.050 66.501 1.000 24.45 ANISOU 678 CA96 ASP 162 - 383 679 C ATOM -471 3228 3466 2597 ASP 96 -7.073 16.589 67.404 1.000 26.51 ANISOU 679 С 96 -170 160 -798 ASP 680 0 MOTA 3370 4047 2656 96 ASP -9.952 15.334 67.334 1.000 24.97 ANISOU 680 0 ASP 96 CB -423 -228 7 7 681 ATOM 3371 3806 2310 -11.411 15.605 67.606 1.000 26.77 96 ANISOU 681 CВ ASP 96 -362 -240 7 1 6 CG ASP 682 MOTA 3566 4334 2272 96 -11.935 16.723 67.388 1.000 33.94 ANISOU 682 CG ASP 96 OD1 ASP 647 204 569 683 ATOM 4733 3267 4894 96 -12.058 14.646 68.083 1.000 32.65 ANISOU 683 OD1 ASP 96 -1032 1446 - 202 OD2 ASP 684 ATOM 4072 4709 3624 96 65.581 1.000 22.21 OD2 ASP ANISOU 684 15.226 -7.25497 TYR -376 -77 -102 N 685 ATOM 2760 3389 2292 14.852 65.583 1.000 23.71 97 ANISOU 685 TYR N -5.835 TYR 97 CA106 644 686 ATOM-27 2987 3542 2480 97 -5.026 15.828 64.743 1.000 23.06 ANISOU 686 TYR CA97 TYR -410 -78 350 С 687 MOTA 3754 2647 97 -3.992 16.327 65.230 1.000 24.29 2363 TYRС ANISOU 687 97 TYR -133 -230 7 688 0 MOTA3178 3845 97 -5.585 13.451 65.035 1.000 28.38 2205 ANISOU 688 TYR 0 97 TYR-450 8 3 2 689 CВ ATOM540 4229 3230 3324 97 -4.132 13.025 65.082 1.000 30.37 TYR CB ANISOU 689 97 TYR -191 6 7 1 CG 690 MOTA 766 4161 4101 97 3278 TYR -3.511 12.691 66.285 1.000 30.19 ANISOU 690 CG CD1 TYR 97 1106 151 951 691 MOTA 4119 4475 2878 CD1 TYR 97 -3.370 12.945 63.922 1.000 29.79 ANISOU 691 97 53 - 253 544 CD2 TYR 692 MOTA 3997 4005 3317 CD2 TYR 97 -2.178 12.294 66.324 1.000 32.77 ANISOU 692 CE1 TYR 97 -68 763 ATOM 693 574 5126 4771 2554 97 CE1 TYR -2.043 12.553 63.955 1.000 32.68 ANISOU 693 CE2 TYR 97 353 323 694 MOTA 403 5087 3793 -1.445 12.228 65.157 1.000 33.00 3536 ANISOU 694 CE2 TYR 97 1066 264 456 97 695 CZTYR MOTA 5622 4284 97 -0.121 11.845 65.156 1.000 42.66 2633 TYR ANISOU 695 CZ97 1161 764 1277 TYR ОН 696 ATOM 8264 5373 97 2572 62.134 1.000 23.20 ANISOU 696 ОН TYR-3.465 16.575 98 SER CB 697 MOTA 105 3587 2766 SER 98 2461 -3.632 15.649 61.078 1.000 26.49 ANISOU 697 CB -154 238 -457 98 SER 698 OG MOTA 3180 3059 -5.694 17.744 61.701 1.000 18.66 3824 98 SER ANISOU 698 OG 98 SER -295 66 1 3 MOTA 699 С 2637 2150 2301 SER 98 17.212 61.413 1.000 20.88 С ANISOU 699 -6.768 98 -945 -249 1 8 1 700 0 SER MOTA 2245 2646 3042 98 16.110 63.511 1.000 23.62 SER ANISOU 700 0 -5.457 98 SER -441 -395 6 0 5 Ν 701 MOTA 2931 3227 2816 98 -4.748 17.143 62.741 1.000 21.31 ANISOU 701 SER Ν 98 SER MOTA 702 CA

- 113 -153 294 2982 133 2430 2687 98 18.891 61.148 1.000 18.68 ANISOU 702 CASER -5.307 99 MET -978 -366 1 0 1 703 N MOTA 1984 2722 2392 MET 99 ANISOU 703 60.075 1.000 17.84 N 19.560 -6.04799 CA MET -945 -212 - 17 704 MOTA 1726 2620 2431 MET 99 60.585 1.000 19.71 ANISOU 704 CA20.779 -6.819 MET 99 CB -679 25 6 4 705 MOTA 2173 2968 2343 99 ANISOU 705 MET 20.392 61.374 1.000 23.68 СВ -8.052 99 MET CG-504 393 489 706 MOTA 3055 3582 99 2360 MET -9.031 21.821 61.911 1.000 22.33 CG ANISOU 706 99 MET 707 SD -522 170 -120 MOTA 2534 3383 2569 99 MET -8.148 22.225 63.419 1.000 36.98 ANISOU 707 SD 99 MET -225 -1904 - 23 708 CE ATOM 3401 4165 6485 99 MET ANISOU 708 CE 19.954 58.973 1.000 17.19 -5.070 99 MET С -960 -194 - 201 709 MOTA 1776 2488 99 2269 MET С ANISOU 709 20.341 59.324 1.000 16.93 -3.964 99 MET -208 - 241 0 710 -367 ATOM 1919 2583 1932 99 ANISOU 710 MET 19.864 57.715 1.000 20.00 100 -5.486 CYS -1753 -358 1 6 6 711 MOTA 1739 100 3178 2683 20.181 56.554 1.000 16.64 CYS ANISOU 711 N 100 -4.645 CACYS -563 4 6 8 712 MOTA -924 1817 2294 100 2213 100 -4.291 18.893 55.813 1.000 17.74 CYS ANISOU 712 CA-765 1 0 5 3 CBCYS MOTA 713 560 2174 2407 100 2161 100 -3.035 18.928 54.552 1.000 33.56 ANISOU 713 CYS CB CYS 714 SG 414 1509 6 0 1 MOTA 3997 100 5244 3511 21.121 55.590 1.000 13.48 CYS ANISOU 714 SG 100 -5.347 CYS 240 - 91 С MOTA 715 -68 1829 100 1879 1415 21.127 55.496 1.000 14.49 С CYS ANISOU 715 100 -6.585 0 CYS -497 -57 1 4 716 MOTA 1673 1952 100 1880 21.921 54.852 1.000 13.35 CYS ANISOU 716 0 101 -4.589 TYR -254 -78 4 9 717 N MOTA 1677 1673 101 1721 101 -5.016 22.753 53.755 1.000 10.27 TYR ANISOU 717 Ν -15 -141 -231 TYR CA718 ATOM 1477 101 926 1498 101 -5.102 24.265 54.124 1.000 13.60 TYR CA ANISOU 718 322 - 236 TYR 719 CB MOTA -48 2027 1513 101 1626 25.025 52.863 1.000 17.31 ANISOU 719 TYR CB 101 -5.498 TYR -158 -103 1 9 3 CG ATOM 720 2694 101 2373 1509 25.068 52.519 1.000 16.38 TYR ÇG ANISOU 720 101 -6.815 CD1 TYR 721 -227 MOTA 190 101 -7.307 25.715 51.412 1.000 17.01 101 2755 714 2993 -86 -416 12 752 3006 CD1 TYR ANISOU 721 CE1 TYR 722 MOTA 101 -4.616 25.679 52.012 1.000 19.51 CE1 TYR ANISOU 722 CD2 TYR -1143 -594 4 7 5 723 MOTA 2847 101 3032 1533 101 -5.065 26.321 50.872 1.000 20.96 CD2 TYR ANISOU 723 112 769 CE2 TYR 724 MOTA 238 3211 101 2802 1949 101 -6.414 26.334 50.568 1.000 22.78 CE2 TYR ANISOU 724 -1228 -919 6 2 4 CZTYR 725 MOTA 3126 2291 101 3238 101 -6.875 26.986 49.442 1.000 23.10 ANISOU 725 CZTYR TYR -129 4 2 9 726 OH MOTA -14 2522 101 3141 3112 101 -4.041 22.518 52.596 1.000 11.25 TYR ANISOU 726 OH-323 103 -252 С TYR 727 MOTA 1654 1398 101 -2.823 22.677 52.787 1.000 12.23 TYR ANISOU 727 С TYR 130 - 20 0 728 MOTA -87 1784 1750 101 1114 22.190 51.405 1.000 11.17 ANISOU 728 TYR 102 -4.542 -220 145 -263 729 Ν SER MOTA 1611 1279 102 1355 21.802 50.235 1.000 10.46 SER ANISOU 729 N 102 -3.752 SER 62 -1 -125 CA730 ATOM 1568 102 1144 1263 20.343 49.908 1.000 13.46 ANISOU 730 CASER 102 -4.027 105 - 301 SER 731 CB ATOM 324 2234 1212 102 1668 19.487 51.025 1.000 16.42 ANISOU 731 CB SER 102 -3.723 SER OG 96 732 -43 MOTA -122 2637 1313 102 2291 ANISOU 732 OG SER



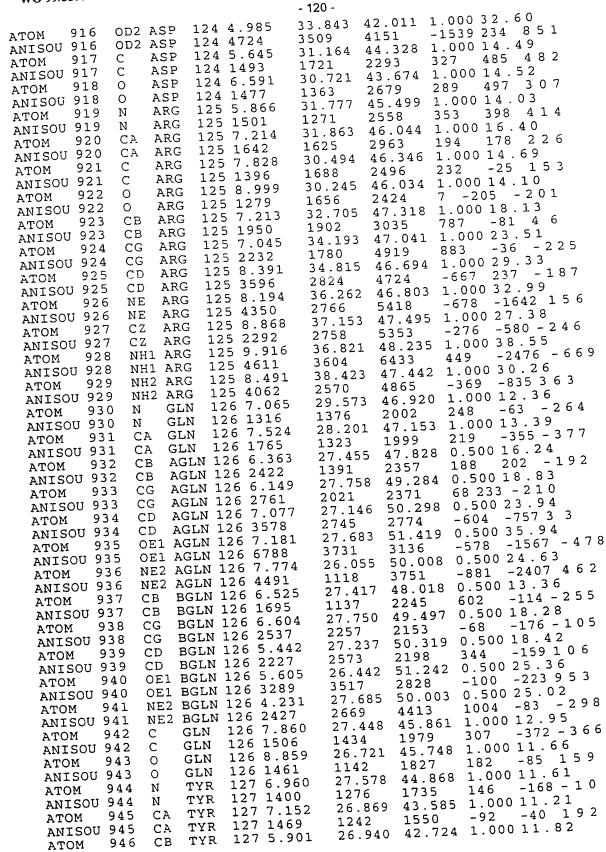


- 116 -111 -11.406 29.717 50.851 1.000 19.41 -386 519 -314 PRO 794 N 2985 MOTA 2110 111 2279 51.705 1.000 19.20 PRO ANISOU 794 N 111 -10.278 29.322 255 - 514 PRO CD795 -417 MOTA 2640 1880 111 2773 111 -12.549 30.252 51.604 1.000 21.47 PRO ANISOU 795 CD728 -635 CAPRO 796 -50 MOTA 3206 1924 111 -12.167 30.007 53.055 1.000 23.63 PRO ANISOU 796 CAPRO 776 - 575 797 CB 334 MOTA 3137 2054 111 3789 111 -10.775 29.535 53.100 1.000 22.33 ANISOU 797 PRO PRO CG -1006 623 -414 798 MOTA 2809 2908 111 2767 PRO 111 -12.828 31.739 51.433 1.000 23.88 ANISOU 798 CG PRO С 79 - 142 - 479 799 MOTA 2049 3887 111 3139 111 -13.919 32.194 51.834 1.000 26.77 ANISOU 799 C PRO -91 -397 PRO 008 0 992 MOTA 3555 2818 111 3800 112 -11.906 32.517 50.872 1.000 25.19 PRO ANISOU 800 0 -856 2 8 2 SER -247 Ν 801 MOTA 3788 2269 112 -12.300 33.919 50.631 1.000 26.43 112 3514 SER ANISOU 801 N 1364 4 5 6 SER CA802 4734 496 MOTA 2655 112 2654 112 -12.506 34.712 51.912 1.000 33.37 SER CAANISOU 802 2582 - 510 803 CB SER ATOM 5895 3663 112 -11.322 34.719 52.688 1.000 36.94 112 3122 SER ANISOU 803 CB 1399 206 -415 SER OG 804 MOTA 5351 2154 112 6530 112 -11.262 34.587 49.723 1.000 26.62 OG SER ANISOU 804 1021 1668 651 С SER 805 ATOM 4956 112 2613 2546 49.414 1.000 22.81 С SER ANISOU 805 112 -10.219 34.029 837 - 400 0 SER 806 800 MOTA 3645 2782 49.279 1.000 28.93 112 2241 SER ANISOU 806 0 113 -11.570 35.802 GLY 1008 1175 1198 807 N ATOM 5108 2947 113 2937 48.365 1.000 30.79 ANISOU 807 GLY N 113 -10.659 36.478 798 1400 GLYCA 808 381 ATOM 5102 3606 113 2992 36.829 49.070 1.000 31.83 ÇА $\operatorname{\mathsf{GLY}}$ ANISOU 808 113 -9.362 897 528 GLY С 809 262 ATOM 4878 3919 113 3297 36.790 48.459 1.000 25.85 GLYANISOU 809 C 113 -8.294 450 - 203 GLY810 0 857 ATOM 2317 4585 113 2920 114 -9.479 37.145 50.365 1.000 29.56 GLY ANISOU 810 0 1104 7 6 0 ASP 811 N 866 MOTA 2877 4868 114 3487 114 -8.257 37.463 51.122 1.000 26.15 N ASP ANISOU 811 1028 1584 5 4 2 CA ASP 812 MOTA 4066 114 3189 2680 114 -8.628 37.937 52.526 1.000 33.81 CA ASP ANISOU 812 1774 1691 - 240 CB ASP 813 MOTA 4569 2697 114 5580 114 -7.904 39.232 52.840 1.000 40.77 ASP ANISOU 813 CВ 693 - 248 ASP CG 814 719 MOTA 4960 3734 114 6798 114 -8.330 40.277 52.295 1.000 48.61 ASP ANISOU 814 CG 1703 931 - 913 OD1 ASP 815 ATOM 9920 2534 114 6014 114 -6.932 39.178 53.622 1.000 54.35 OD1 ASP ANISOU 815 -868 495 1602 OD2 ASP 816 MOTA 7783 7609 114 5258 114 -7.310 36.281 51.231 1.000 23.05 OD2 ASP ANISOU 816 ASP 1874 3 4 0 С 444 MOTA 817 4033 2102 114 -6.111 36.371 50.955 1.000 22.05 С ASP ANISOU 817 1411 - 461 ASP 818 0 131 3677 MOTA 2277 115 -7.854 35.160 51.637 1.000 23.21 ASP ANISOU 818 0 -130 1293 - 228 PHE 819 N MOTA 3984 1890 115 2945 115 -7.120 33.896 51.690 1.000 19.93 PHE ANISOU 819 N -198 655 -294 PHE CA820 MOTA 3102 1908 115 2562 32.792 52.157 1.000 19.49 PHE CAANISOU 820 115 -8.085 64 881 - 314 CB PHE 821 ATOM 3275 1754 115 2378 31.445 52.540 1.000 17.25 PHE ANISOU 821 CB 115 -7.523 348 - 695 PHE CG 822 -56 MOTA 2912 1589 115 2053 30.951 53.833 1.000 19.00 PHE ANISOU 822 CG 115 -7.637 CD1 PHE 73 496 -683 823 MOTA 2950 1539 115 2728 115 -6.868 30.634 51.615 1.000 17.88 CD1 PHE ANISOU 823 CD2 PHE 824 ATOM

- 117 -7 298 -810 2927 1931 29.711 54.163 1.000 20.25 115 1933 CD2 PHE ANISOU 824 115 -7.100 341 -575 CE1 PHE 317 825 3042 115 2825 1825 51.955 1.000 19.11 CE1 PHE ANISOU 825 29.412 115 -6.338 351 -885 CE2 PHE 336 3237 826 MOTA 2158 115 1865 53.233 1.000 19.39 CE2 PHE ANISOU 826 115 -6.452 28.936 248 -669 PHE CZ320 ATOM 827 3390 1910 115 2068 33.624 50.327 1.000 17.86 PHE CZANISOU 827 115 -6.506 PHE 61 344 1 6 828 С 2878 ATOM 1945 115 1964 33.315 50.271 1.000 17.34 PHE ANISOU 828 C 115 -5.324 -132 179 157 0 PHE 829 2613 MOTA 2107 115 1868 116 -7.310 33.683 49.263 1.000 18.21 PHE ANISOU 829 0 281 6 2 GLU N 547 830 3065 MOTA 1934 116 1921 116 -6.848 33.387 47.907 1.000 19.99 GLU ANISOU 830 Ν GLU 81 231 2 2 2 CA831 MOTA 2618 2851 116 2128 116 -7.968 33.605 46.884 1.000 18.61 GLU ANISOU 831 CA2 7 0 GLU CB 832 3060 231 MOTA 1952 116 2058 116 -7.398 33.378 45.482 1.000 18.61 ANISOU 832 CВ GLU -32 - 33 GLU CG 295 MOTA 833 2971 2288 116 1813 33.230 44.412 1.000 22.40 GLU CG ANISOU 833 116 -8.442 -122 -278 - 91 GLU CD 834 3410 MOTA 3193 33.272 44.678 1.000 30.82 116 1908 GLU ANISOU 834 CD116 -9.654 -414 - 24 OE1 GLU 273 835 5452 MOTA 4465 116 1793 33.063 43.225 1.000 30.24 OE1 GLU ANISOU 835 116 -8.085 -658 3 2 7 OE2 GLU 382 836 3026 MOTA 5132 116 3333 1.000 18.82 OE2 GLU 116 -5.620 34.211 47.535 ANISOU 836 119 487 GLU 294 С 837 2990 ATOM 2069 33.701 47.049 1.000 17.41 116 2090 ANISOU 837 С GLU 116 -4.605 45 259 282 GLU 0 838 2606 MOTA 1780 116 2228 35.508 47.777 1.000 21.02 0 GLU ANISOU 838 117 -5.660 220 9 0 ARG 839 N 408 3487 MOTA 2185 117 2313 36.420 47.431 1.000 21.35 ARG ANISOU 839 N 117 -4.560 147 - 31 ARG CA466 840 3976 MOTA 117 2337 1800 36.054 48.192 1.000 20.52 ARG ANISOU 840 CA117 -3.291 288 - 10 ARG С 353 841 3380 MOTA 117 -2.186 35.969 47.636 1.000 18.96 2124 117 2292 ARG С ANISOU 841 318 231 ARG 0 MOTA 842 1664 3316 37.885 47.693 1.000 25.59 117 2223 ARG 0 ANISOU 842 117 -4.971 1882 6 3 2 ARG СB 929 843 4587 ATOM 38.908 47.478 1.000 32.57 1900 117 3237 CB ARG ANISOU 843 117 -3.881 1083 6 2 3 ARG -281 CG 5237 844 MOTA 1925 117 5212 117 -4.325 40.323 47.859 1.000 36.56 ARG ANISOU 844 CG 1774 6 6 3 ARG 149 CDATOM 845 5724 2157 117 6009 117 -5.162 40.335 49.056 1.000 44.43 ANISOU 845 ARG CD 2344 - 15 ARG ΝE 846 5940 MOTA 40.501 50.306 1.000 45.48 3742 117 7200 ARG NE ANISOU 846 117 -4.763 -370 2388 - 283 ARG CZ847 MOTA 6054 4804 117 -3.484 40.683 50.619 1.000 53.21 ARG CZANISOU 847 -2543 2487 3 5 4 NH1 ARG 848 6900 MOTA 117 6867 40.487 51.301 1.000 50.00 6451 NH1 ARG ANISOU 848 117 -5.647 2433 - 1534 NH2 ARG 224 849 6220 ATOM 6511 35.832 49.493 1.000 19.30 117 6265 NH2 ARG ANISOU 849 118 -3.439 407 - 645 ILE 128 850 N MOTA 3221 1838 118 2275 50.331 1.000 18.25 ILE ANISOU 850 N 35.527 118 -2.275 78 530 - 449 ILE CA851 MOTA 2811 1745 51.820 1.000 18.24 118 2376 ANISOU 851 ILE CA35.597 118 -2.665 906 - 306 ILE ATOM 852 CB 346 3003 1726 118 2201 52.732 1.000 18.49 ANISOU 852 ILE CB 34.851 -202 308 -530 118 -1.712 CG2 ILE 853 2792 MOTA 2158 118 2077 37.031 52.368 1.000 24.69 CG2 ILE ANISOU 853 118 -2.877 1382 - 414 CG1 ILE 284 MOTA 854 3136 1808 118 4436 CG1 ILE ANISOU 854

- 118 -37.025 53.582 1.000 29.63 118 -3.786 1258 - 1068 CD1 ILE 189 855 1994 MOTA 118 6169 3096 49.959 1.000 15.65 CD1 ILE ANISOU 855 34.172 118 -1.692 573 - 117 C ILE -89 MOTA 856 2082 1549 49.802 1.000 14.59 118 2316 ILE C ANISOU 856 34.035 118 -0.463 ILE 16 286 2 1 4 0 857 2051 ATOM 1255 118 2240 49.784 1.000 14.44 ILE ANISOU 857 0 33.139 119 -2.523 47 128 - 7 1 TRP 858 N 1771 MOTA 1592 119 2125 31.795 49.518 1.000 13.68 TRP ANISOU 858 N 119 -2.010 220 4 0 TRP CA. -61 859 1957 MOTA 1529 119 1712 30.755 49.932 1.000 14.93 TRP ANISOU 859 CA119 -3.089 TRP -234 295 - 35 СВ 860 2123 MOTA 1729 119 1819 30.482 51.420 1.000 16.19 TRP CB ANISOU 860 119 -2.864 -168 582 167 TRP CG 861 2146 MOTA 2364 119 -2.116 29.430 51.993 1.000 20.41 119 1640 TRP CG ANISOU 861 523 405 CD2 TRP MOTA 862 2151 202 2414 119 3189 29.580 53.392 1.000 19.84 CD2 TRP ANISOU 862 119 -2.177 1 3 7 CE2 TRP 234 863 -439 2184 ATOM 119 3536 1818 119 -1.390 28.357 51.456 1.000 23.94 CE2 TRP ANISOU 863 126 400 CE3 TRP 864 2068 561 MOTA 1647 119 5382 31.223 52.460 1.000 20.05 CE3 TRP ANISOU 864 119 -3.340 CD1 TRP -9 189 -139 865 2069 MOTA 2343 119 3207 30.689 53.649 1.000 20.32 CD1 TRP ANISOU 865 119 -2.938 -68 -185 NE1 TRP -96 866 ATOM 2726 2188 119 2806 54.281 1.000 22.12 NE1 TRP ANISOU 866 119 -1.547 28.714 -17 105 2 2 CZ2 TRP 867 2078 ATOM 2256 119 4071 52.332 1.000 21.52 CZ2 TRP ANISOU 867 27.490 119 -0.761 -193 1 9 7 CZ3 TRP 868 311 MOTA 1794 2168 119 4214 53.715 1.000 24.34 CZ3 TRP ANISOU 868 27.674 119 -0.847 148 183 CH2 TRP 329 869 1850 MOTA2047 48.095 1.000 14.27 119 5349 CH2 TRP ANISOU 869 31.634 119 -1.521 -187 334 -65 TRP С ATOM 870 1985 1259 119 2180 30.865 47.855 1.000 14.73 TRP ANISOU 870 С 119 -0.569 362 101 TRP 0 -67 871 1946 MOTA 1653 32.325 47.116 1.000 13.99 119 1996 TRP ANISOU 871 0 120 -2.109 627 - 137 THR N 106 872 MOTA 1848 1237 32.275 45.762 1.000 15.19 120 2231 THR ANISOU 872 N 120 -1.541 9 435 - 242 THR CA873 1774 MOTA 32.983 44.787 1.000 16.41 2093 120 1903 THR CA ANISOU 873 120 -2.492 -331 152 6 THR CB 874 1995 MOTA 2304 32.297 44.766 1.000 18.53 120 1934 THR ANISOU 874 CB 120 -3.738 -236 195 407 OG1 THR 875 MOTA 2288 2863 32.906 43.358 1.000 18.02 120 1891 OG1 THR ANISOU 875 120 -1.974 322 318 CG2 THR 324 876 MOTA 2108 2602 120 2135 32.870 45.727 1.000 14.19 CG2 THR ANISOU 876 120 -0.145 87 285 - 167 THR С 877 MOTA 1475 2050 120 1868 32.299 45.078 1.000 13.62 THR ANISOU 877 С 120 0.756 354 217 THR 878 301 1620 MOTA 1692 46.429 1.000 14.55 120 1864 THR ANISOU 878 0 33.962 121 0.114 175 - 67 304 N GLN 879 2136 MOTA 1672 46.483 1.000 15.80 121 1721 N GLN ANISOU 879 34.548 121 1.459 -119 3 6 2 GLN CA-18 880 2271 ATOM 1666 121 2067 47.176 1.000 13.73 GLN ANISOU 880 CA33.642 121 2.465 18 1 1 4 GLN С -30 881 1806 MOTA 1665 46.685 1.000 15.36 121 1747 GLN С ANISOU 881 33.452 121 3.603 48 360 - 4 4 GLN 0 882 2084 MOTA 1688 121 2063 47.154 1.000 18.85 ANISOU 882 0 GLN 35.918 121 1.315 CB -5 3 5 6. GLN-73 883 MOTA 3200 1426 121 2537 36.558 47.543 1.000 18.88 GLN CB ANISOU 883 121 2.639 -248 GLN CG 59 9 884 MOTA 2878 1788 121 2507 36.936 46.337 1.000 20.70 GLNCG ANISOU 884 121 3.468 GLN CD 885 ATOM

- 119 --85 231 -373 3142 2138 37.088 45.224 1.000 22.47 121 2584 CD GLN ANISOU 885 121 2.935 OE1 GLN 886 -245 3019 2822 121 2695 37.101 46.522 1.000 25.22 OE1 GLN ANISOU 886 121 4.779 NE2 GLN -131 1385 127 887 ATOM 3811 3344 121 2426 NE2 GLN 1.000 12.26 ANISOU 887 33.054 48.299 122 2.081 TYR 99 - 55 - 258 Ν 888 MOTA 1399 1514 122 1747 32.102 49.050 1.000 13.18 TYR N ANISOU 888 122 2.896 -20 -253 - 160 CA TYR 889 MOTA 1464 1643 122 1901 31.724 50.364 1.000 13.78 TYP ANISOU 889 С¥ 122 2.211 TYR 48 - 28890 CB 116 ATOM 1756 1435 122 2045 30.808 51.282 1.000 14.22 ANISOU 890 TYR CB 122 2.994 TYR 68 1 0 1 CG 891 101 ATOM 1758 1681 122 1966 TYR31.120 51.722 1.000 17.48 CG ANISOU 891 122 4.271 CD1 TYR -5 4 2 0 892 149 MOTA 2882 1972 122 1788 30.284 52.576 1.000 18.55 CD1 TYR ANISOU 892 122 5.003 -404 2 5 1 CE1 TYR 893 102 ATOM 2868 2050 122 2131 29.619 51.731 1.000 20.72 CE1 TYR ANISOU 893 122 2.445 -519 -1524 3 2 3 CD2 TYR 3197 894 ATOM1366 122 3308 28.773 52.574 1.000 25.40 CD2 TYR ANISOU 894 122 3.140 -2084 873 CE2 TYR 895 -782 4067 ATOM 1812 122 3772 29.101 52.992 1.000 20.93 CE2 TYR ANISOU 895 122 4.413 -1145 3 1 3 TYR 896 CZ-96 MOTA 3224 1742 122 2985 28.230 53.826 1.000 29.87 TYR ANISOU 896 CZ122 5.068 -680 -3078 621 TYR OH897 MOTA 4522 1998 122 4830 30.876 48.209 1.000 12.33 ANISOU 897 TYR OH 122 3.218 TYR89 -218 8 8 898 С 1439 MOTA 1412 122 1833 30.507 48.117 1.000 14.25 ANISOU 898 С TYR 122 4.395 -242 2 1 6 TYR 899 0 339 ATOM 1656 1861 122 1896 30.269 47.573 1.000 11.28 ANISOU 899 TYR 0 123 2.224 6 -151 185 PHE N 900 MOTA 1041 1297 123 1950 29.151 46.665 1.000 12.08 ANISOU 900 N PHE 123 2.482 64 - 60 2 6 PHE CA901 MOTA 1640 1219 123 1731 28.719 46.024 1.000 13.86 ANISOU 901 PHE CA123 1.139 -104 -276 - 82 PHE 902 CB ATOM 1666 1550 123 2048 27.516 45.099 1.000 14.44 PHE ANISOU 902 CB 123 1.311 -475 - 9 4 PHE CG ATOM 903 1637 142 1677 123 2173 26.234 45.614 1.000 13.64 ANISOU 903 PHE CG 123 1.281 -702 - 236 CD1 PHE 904 -42 MOTA 1764 1563 123 1857 27.664 43.729 1.000 13.81 CD1 PHE ANISOU 904 123 1.511 -420 -295 -248 CD2 PHE 905 MOTA 1634 2164 25.141 44.795 1.000 17.16 123 1450 ANISOU 905 CD2 PHE 123 1.468 -855 - 644 CE1 PHE 906 130 ATOM 2418 1819 123 2282 26.559 42.916 1.000 18.31 ANISOU 906 CE1 PHE 123 1.715 -1053 172 -845 CE2 PHE 907 MOTA 2201 2657 123 2098 25.295 43.445 1.000 16.71 CE2 PHE ANISOU 907 123 1.706 -306 -1077 PHE CZ908 -36 MOTA 2526 2382 123 1442 29.511 45.581 1.000 13.48 PHE **ANISOU 908** CZ123 3.489 157 1 8 PHE С 909 1645 236 MOTA 123 2004 1472 28.768 45.242 1.000 13.07 PHE С ANISOU 909 123 4.424 42 - 78 - 172 PHE 910 0 MOTA 1876 1498 123 1591 30.684 44.948 1.000 13.83 PHE ANISOU 910 124 3.294 51 207 288 ASP MOTA 911 N 2189 1575 124 1490 31.036 43.861 1.000 13.75 ASP N ANISOU 911 124 4.207 398 344 CAASP 458 912 MOTA 2389 1330 124 1505 1.000 18.95 ASP ANISOU 912 CA43.242 32.352 124 3.708 -63 926 CB ASP 656 913 2580 MOTA 1970 124 2650 41.989 1.000 27.54 ANISOU 913 ASP CB 32.708 124 4.470 -123 939 880 ASP CG 914 MOTA 2099 3036 124 5327 1.000 37.04 ASP ANISOU 914 CG41.023 31.904 124 4.541 2616 - 331 OD1 ASP 915 108 MOTA 4485 3225 124 6362 OD1 ASP ANISOU 915



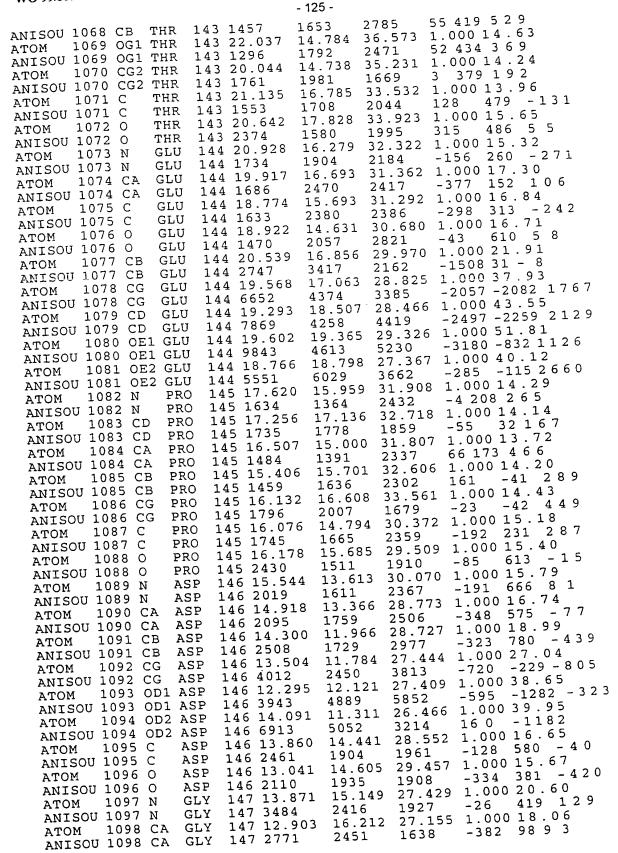
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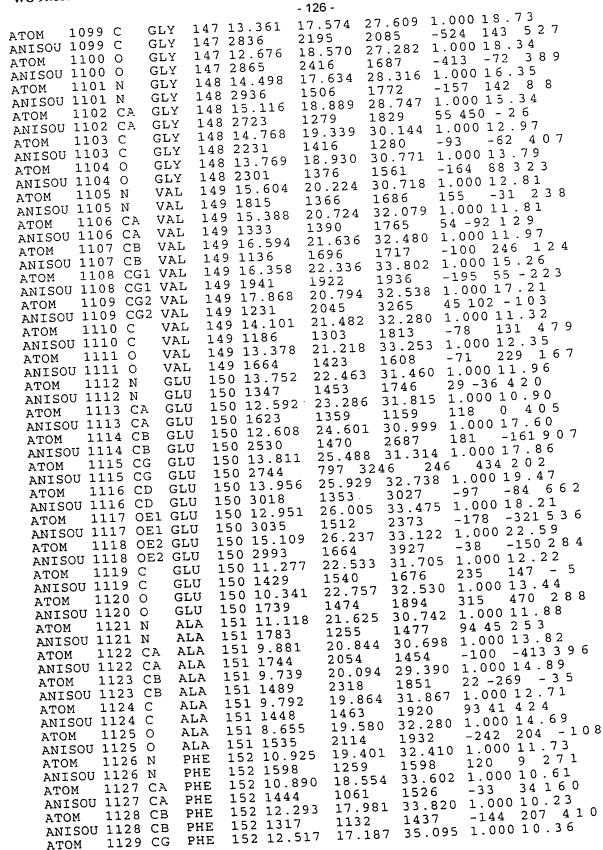
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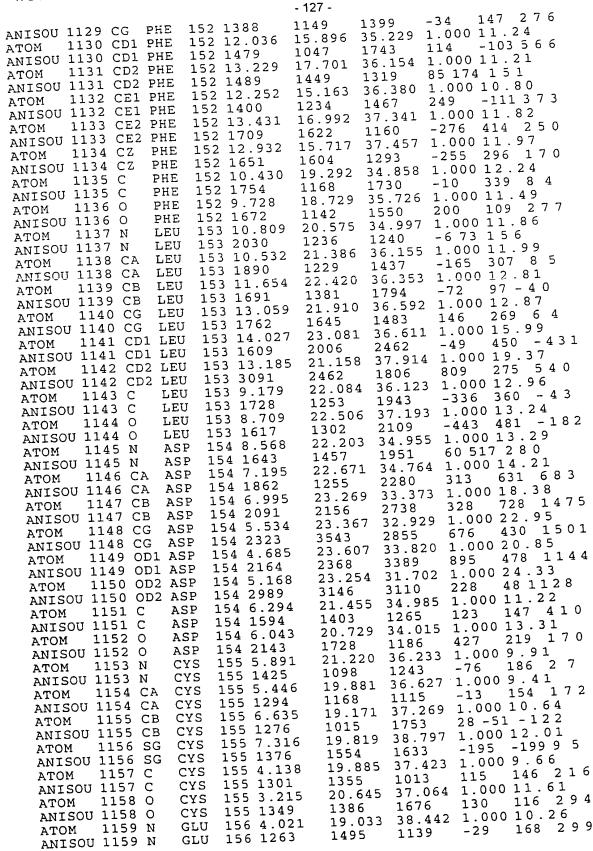
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ANISOU 1038 0 ARG 139 22.184 20.816 37.614 1.000 13.20	
ATOM 1039 N ARG 139 1432 2046 1561 -155 219 31 7	
ANISO 1040 CA ARG 139 23.397 21.372 37.003 1.37 502 447	
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ATOM 1041 C ARG 139 24.05 2101 2235 -158 324 116	
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ATOM 1042 O ARG 139 1628 2581 2688 10 000 19 67	
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7000 1001 CA 4424 ==:	
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ANDM 1065 0 GLY 142 24.654 15.824 33.37 57.798 1 6 3	
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26.134 49.640 1.000 13.33

21.846 49.868 1.000 11.24

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1184 CA

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ANISOU 1188 CD2 LEU

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1188 CD2 LEU

ANISOU 1184 CA

ANISOU 1185 CB

ANISOU 1186 CG

ANISOU 1189 C

ATOM

MOTA

MOTA

MOTA

MOTA

MOTA

MOTA

- 129 --328 34 - 269 1457 2395 LEU 159 1354 21.385 51.010 1.000 14.59 ANISOU 1190 O 160 1.013 -390 -128 - 224 ARG 1191 N MOTA 1239 2569 160 1737 21.030 52.153 1.000 13.94 ANISOU 1191 N ARG 160 0.158 -137 9 2 ARG 157 1192 CA ATOM1402 2631 160 1265 19.528 52.343 1.000 18.20 ANISOU 1192 CA ARG 160 0.161 -301 32 1 9 3 ARG 1193 CB 2338 2645 160 1932 160 -0.423 18.661 51.252 1.000 25.12 ANISOU 1193 CB ARG -653 -787 2 3 ARG 1194 CG MOTA 3191 2902 160 3451 160 -0.765 17.301 51.831 1.000 31.98 ANISOU 1194 CG ARG ARG -1994 -905 3 2 1 1195 CD MOTA 3729 3598 160 4825 160 -1.284 16.322 50.896 1.000 26.15 ARG ANISOU 1195 CD -739 -1056 310 ARG 1196 NE 2957 3587 MOTA 160 -0.970 15.044 50.779 1.000 25.30 160 3392 ANISOU 1196 NE ARG 94 - 785 295 ARG 1197 CZ 3028 ATOM3390 160 3195 160 -0.063 14.433 51.552 1.000 31.26 ANISOU 1197 CZ ARG -629 -1089 2054 1198 NH1 ARG ATOM 4080 160 3654 4142 160 -1.572 14.308 49.850 1.000 28.82 ANISOU 1198 NH1 ARG -966 - 90 1199 NH2 ARG 160 4020 3122 3807 -13 -966 -160 0.649 21.669 53.447 1.000 15.12 ANISOU 1199 NH2 ARG -66 125 ARG 1200 C 160 1649 2863 104 1232 ATOM21.556 53.863 1.000 17.09 ANISOU 1200 C ARG 160 1.804 -400 74 -812 ARG 1201 0 ATOM 1791 3411 160 1291 161 -0.258 22.369 54.114 1.000 14.95 ARG ANISOU 1201 O -253 -8 -146 PHE 1202 N MOTA 2506 1660 161 1512 161 -0.036 22.949 55.427 1.000 13.27 ANISOU 1202 N PHE -9 -249 - 41 1203 CA PHE ATOM1760 161 1600 1681 161 -0.587 24.381 55.472 1.000 16.82 ANISOU 1203 CA PHE 1204 CB PHE 384 MOTA 2851 1947 161 -0.317 25.109 56.771 1.000 22.56 161 1594 ANISOU 1204 CB PHE -1067 PHE 1205 CG -39 MOTA 3684 161 -1.175 25.010 57.849 1.000 26.03 2424 ANISOU 1205 CG PHE 1106 - 702 1206 CD1 PHE 267 MOTA3620 2919 25.901 56.885 1.000 25.34 161 3353 ANISOU 1206 CD1 PHE 161 0.822 -179 -161 -738 1207 CD2 PHE 161 2353 4011 MOTA 3265 161 -0.943 25.660 59.051 1.000 30.50 ANISOU 1207 CD2 PHE -972 1456 - 620 1208 CE1 PHE \mathtt{MOTA} 26.553 58.080 1.000 26.10 3481 161 4784 ANISOU 1208 CE1 PHE 161 1.061 -129 281 -1127 1209 CE2 PHE 4302 ATOM3067 161 2546 26.438 59.164 1.000 30.06 ANISOU 1209 CE2 PHE 161 0.199 774 - 677 1210 CZ PHE -152 MOTA 4386 3197 161 -0.737 22.073 56.447 1.000 13.93 PHE ANISOU 1210 CZ -334 -277 - 240 PHE 1211 C MOTA 1503 PHE 161 -1.916 21.843 56.270 1.000 18.26 1946 ANISOU 1211 C -744 -399 4 7 5 1212 0 MOTA PHE 161 2000 ARG 162 -0.090 21.631 57.503 1.000 16.29 3277 ANISOU 1212 O -937 -523 7 7 1213 N MOTA 1610 162 2063 2516 162 -0.635 20.719 58.483 1.000 15.62 ARG ANISOU 1213 N -519 -266 7 6 1214 CA ARG MOTA 1650 2512 162 1772 162 -0.476 21.312 59.890 1.000 17.48 ANISOU 1214 CA ARG -603 -186 - 76 ARG 1215 C 1656 MOTA 162 1855 3131 21.734 60.251 1.000 17.23 ANISOU 1215 C ARG 162 0.609 -771 -42 -160 1216 0 ARG ATOM 1557 3063 162 1928 19.374 58.458 1.000 21.99 ANISOU 1216 O ARG 162 0.081 -272 -737 - 22 ARG 1217 CB MOTA 2727 2318 162 -0.573 18.322 59.348 1.000 26.07 ANISOU 1217 CB ARG 655 280 1218 CG ARG MOTA 4041 2375 162 3488 16.896 58.886 1.000 25.85 ANISOU 1218 CG ARG 162 -0.231 -2239 1219 CD ARG 418 MOTA 4495 162 -0.943 15.916 59.698 1.000 28.83 2221 162 3106 ANISOU 1219 CD ARG -181 332 -177 ARG 1220 NE 4139 2437 162 4379 ARG ANISOU 1220 NE

- 130 -14.638 59.879 1.000 27.99 162 -0.642 -179 962 8 4 1221 CZ ARG MOTA 3868 2497 162 4271 59.273 1.000 26.61 ANISOU 1221 CZ ARG 14.119 162 0.429 -126 - 268 1222 NH1 ARG -91 3167 3742 162 3200 60.658 1.000 34.20 ANISOU 1222 NH1 ARG 13.883 162 -1.408 -986 702 780 1223 NH2 ARG 5663 MOTA 3522 162 3807 60.622 1.000 16.77 ANISOU 1223 NH2 ARG 163 -1.570 21.296 -484 -1948 4 1224 N TYR 1705 MOTA 21.749 61.997 1.000 16.73 2865 163 1803 TYRANISOU 1224 N 163 -1.627 -692 -51 4 0 TYR 1225 CA MOTA 1766 2770 163 1819 22.804 62.116 1.000 18.99 TYR ANISOU 1225 CA 163 -2.712 -427 -303 -214 TYR 1226 CB 2175 MOTA 163 2479 2560 163 -3.173 23.206 63.488 1.000 23.52 ANISOU 1226 CB TYR -335 -868 TYR ATOM 1227 CG -16 2544 163 2573 3821 23.848 64.367 1.000 31.80 ANISOU 1227 CG TYR163 -2.316 -1151 304 -2338 1228 CD1 TYR 3466 MOTA 5005 163 3613 ANISOU 1228 CD1 TYR 24.222 65.625 1.000 40.74 -1906 976 -3116 163 -2.731 1229 CE1 TYR 3950 5676 163 5855 22.965 63.931 1.000 32.55 ANISOU 1229 CE1 TYR 163 -4.459 -1066 639 -2340 1230 CD2 TYR 3408 ATOM 5654 163 -4.902 23.332 65.189 1.000 42.99 163 3307 ANISOU 1230 CD2 TYR -2352 1989 -2949 1231 CE2 TYR 6630 4080 ATOM 163 5626 163 -4.017 23.960 66.025 1.000 42.52 ANISOU 1231 CE2 TYR -1721 1943 - 3714 TYR 1232 CZ 4075 MOTA 163 6281 5799 163 -4.380 24.351 67.274 1.000 48.87 ANISOU 1232 CZ TYR -269 1801 - 3052 1233 OH TYR3569 MOTA 6831 163 -1.935 20.551 62.896 1.000 17.90 ANISOU 1233 OH TYR-894 -465 -173 TYR1234 C 1575 MOTA 2353 163 -2.933 19.858 62.653 1.000 18.12 163 2872 ANISOU 1234 C TYR -732 -615 6 7 TYR 1235 0 2060 MOTA 2130 163 2694 PHE 164 -1.112 20.326 63.898 1.000 18.32 ANISOU 1235 O -614 -402 - 90 1236 N MOTA 1826 164 2516 2621 164 -1.340 19.381 64.984 1.000 23.44 ANISOU 1236 N PHE -727 -669 2 1 9 PHE 1237 CA ATOM2038 2692 164 -0.073 18.617 65.327 1.000 26.02 164 4176 ANISOU 1237 CA PHE -459 -822 3 7 9 PHE 1238 CB 2470 . ATOM 2824 164 4594 17.669 64.231 1.000 29.00 ANISOU 1238 CB PHE 164 0.407 -427 - 254 1239 CG PHE -518 3263 ATOM 164 4118 3639 18.118 63.205 1.000 27.11 ANISOU 1239 CG PHE164 1.224 -198 -821 4 1240 CD1 PHE 3249 ATOM 4013 164 3040 16.332 64.240 1.000 28.37 ANISOU 1240 CD1 PHE 164 0.051 30 - 641241 CD2 PHE 3704 472 MOTA 3139 164 3935 17.248 62.223 1.000 28.13 ANISOU 1241 CD2 PHE 164 1.657 1242 CE1 PHE -229 6 -43 MOTA 4034 164 2730 3926 15.464 63.250 1.000 31.71 ANISOU 1242 CE1 PHE 164 0.459 -293 657 -383 1243 CE2 PHE MOTA 3694 3635 164 4719 15.924 62.234 1.000 30.26 ANISOU 1243 CE2 PHE 164 1.276 0 300 1 2 6 PHE 1244 CZ 3862 MOTA 3808 164 3827 20.160 66.228 1.000 24.65 ANISOU 1244 CZ PHE 164 -1.775 -1025 -455 3 7 1245 C PHE 1777 MOTA 20.713 66.885 1.000 25.54 4049 164 3541 ANISOU 1245 C PHE -921 -440 - 257 164 -0.889 PHE 1246 0 MOTA 2019 4167 164 3520 20.293 66.527 1.000 32.24 PHE ANISOU 1246 O -1894 266 -680 165 -3.058 1247 N PRO MOTA 3513 5095 165 -3.486 21.012 67.720 1.000 32.98 165 3641 ANISOU 1247 N PRO -1271 397 - 322 1248 CA PRO MOTA 3225 20.429 68.986 1.000 38.48 5737 165 3570 PRO ANISOU 1248 CA 165 -2.854 -1872 40 3 4 3 PRO 1249 C 3457 MOTA 19.230 69.034 1.000 53.87 6808 165 4355 ANISOU 1249 C PRO 165 -2.551 -959 692 1750 PRO 1250 0 3507 MOTA 7012 165 9948 20.820 67.769 1.000 37.76 PRO ANISOU 1250 O 165 -5.001 PRO 1251 CB MOTA

- 131 -4227 -1488 380 -717 6479 165 3640 165 -5.417 20.048 66.569 1.000 36.16 PRO ANISOU 1251 CB -518 -349 - 398 PRO 1252 CG 3948 6449 165 -4.197 19.816 65.734 1.000 35.70 PRO ANISOU 1252 CG -1656 -5 -604 1253 CD PRO 3828 MOTA 6296 66.987 1.000 36.23 165 3440 ANISOU 1253 CD PRO 8.087 178 4.459 1216 1175 LEU -26 1254 N 5918 MOTA 3338 178 4509 66.116 1.000 28.63 LEU ANISOU 1254 N 9.117 178 4.994 1344 4 0 1 LEU 377 1255 CA 4312 MOTA 3170 178 3397 ANISOU 1255 CA 65.027 1.000 30.08 LEU 8.534 178 5.882 752 -620 1256 CB LEU 760 4688 MOTA 3245 178 3497 65.348 1.000 29.43 ANISOU 1256 CB LEU 7.948 178 7.245 371 - 979 LEU 1257 CG 4674 667 ATOM 2950 LEU 178 3557 64.073 1.000 32.13 ANISOU 1257 CG 7.367 178 7.859 586 810 - 790 1258 CD1 LEU 4524 4713 MOTA 178 2972 8.964 65.937 1.000 41.71 ANISOU 1258 CD1 LEU 178 8.208 -1656 -1154 1259 CD2 LEU 356 6850 MOTA 3695 9.909 65.420 1.000 27.18 178 5303 ANISOU 1259 CD2 LEU 178 3.885 -175 1776 8 3 3 LEU 1260 C 4686 ATOM 178 2.845 9.351 65.086 1.000 39.60 3534 LEU ANISOU 1260 C -1253 1290 2183 LEU 1261 0 8016 MOTA 4624 11.200 65.160 1.000 25.65 178 2407 LEU ANISOU 1261 0 179 4.128 -216 878 741 ARG 1262 N MOTA 4089 179 2220 3437 11.973 64.321 1.000 25.04 ANISOU 1262 N ARG 179 3.231 69 641 1 5 1263 CA ARG 4365 MOTA 3289 ANISOU 1263 CA ARG 11.572 62.852 1.000 24.51 179 1860 179 3.297 39 99 - 8 9 ARG 1264 C 4434 ATOM 2721 179 2158 11.687 62.139 1.000 28.60 ANISOU 1264 C ARG 179 2.295 -332 - 256 1265 0 ARG 441 MOTA 179 2545 5079 3242 13.480 64.451 1.000 28.58 ANISOU 1265 O ARG 179 3.517 179 3980 -110 -843 5 7 1266 CB ARG ATOM 3561 14.092 65.724 1.000 30.01 3317 ANISOU 1266 CB ARG 57 - 957 - 3.72 179 2.936 ARG 1267 CG 3862 MOTA3725 15.570 65.757 1.000 31.51 179 3817 ANISOU 1267 CG ARG 179 3.307 90 -1514 - 338 1268 CD ARG 3840 ATOM 3675 179 4457 16.126 67.058 1.000 37.82 ARG ANISOU 1268 CD 179 2.925 -310 - 1 5 ARG 1269 NE 153 4144 MOTA 3190 17.425 67.292 1.000 39.43 179 7035 ANISOU 1269 NE ARG 179 2.897 -479 580 400 ARG 1270 CZ 3532 MOTA 3029 18.286 66.331 1.000 59.73 179 8420 ANISOU 1270 CZ ARG -1045 3177 1722 179 3.213 1271 NH1 ARG MOTA 4676 6273 179 11745 17.896 68.457 1.000 33.13 ANISOU 1271 NH1 ARG 275 -1463 -173 179 2.548 1272 NH2 ARG 3094 3832 MOTA 179 5661 11.099 62.424 1.000 21.43 ANISOU 1272 NH2 ARG -395 108 -222 180 4.455 MET 1273 N 3674 MOTA 2457 180 2013 180 4.695 10.539 61.108 1.000 20.07 MET ANISOU 1273 N 3315 -349 -300 1 5 1 MET 1274 CA ATOM 1965 61.182 1.000 17.33 180 2346 MET ANISOU 1274 CA 180 2340 180 5.802 9.482 180 2251 2080 -332 -86 337 MET 1275 C 2254 61.677 1.000 18.52 180 2251 180 2251 180 6.894 9.757 180 2237 2019 MET ANISOU 1275 C -398 -79 5 2 MET 1276 0 2781 MOTA 180 5.041 11.646 60.136 1.000 22.64 MET ANISOU 1276 O -197 -549 683 MET 1277 CB MOTA 2321 180 2571 11.367 58.678 1.000 27.90 ANISOU 1277 CB \mathtt{MET} 180 5.065 -453 -654 9 1 3 MET 1278 CG 3588 MOTA 3095 12.838 57.629 1.000 25.01 180 3918 ANISOU 1278 CG MET -399 124 851 180 4.945 MET 1279 SD MOTA 3626 2942 12.010 56.147 1.000 37.00 180 2936 ANISOU 1279 SD MET -258 -2680 1204 180 4.385 MET 1280 CE 4690 MOTA 3450 60.680 1.000 16.99 180 5917 MET ANISOU 1280 CE 8.295 ALA 181 5.467 -558 2 9 9 1281 N -90 2174 MOTA 2139 181 2144 ALA ANISOU 1281 N

- 132 -7.168 60.676 1.000 16.12 1282 CA ALA 181 6.396 -171 -343 6 0 2 1890 1958 60.279 1.000 20.24 ALA 181 2275 ANISOU 1282 CA 5.891 -648 694 106 181 5.668 ALA 1283 CB 2673 2158 59.738 1.000 15.43 ALA 181 2857 ANISOU 1283 CB 7.409 ALA 181 7.576 -315 -369 4 3 2 1284 C ATOM 1925 1717 58.783 1.000 15.49 ALA 181 2223 ANISOU 1284 C ALA 181 7.458 8.198 -173 -296 4 3 4 1285 0 MOTA 1858 1761 181 2268 59.986 1.000 16.03 ALAANISOU 1285 O 6.733 182 8.698 5.802 61.101 1.000 19.61 2908 2221 -210 -306 13 6.907 59.076 1.000 14.78 32 - 78 5 3 1 PRO 1286 N PRO 182 2517 1745 MOTA ANISOU 1286 N PRO 182 8.983 -210 -306 1 2 4 0 1287 CD ATOM PRO 182 2321 ANISOU 1287 CD PRO 182 9.865 -101 -86 299 1288 CA 1336 1706 MOTA PRO 182 10.914 5.948 59.649 1.000 16.20 ANISOU 1288 CA -251 7 7 1289 CB 1978 1607 PRO 182 10.479 5.713 61.066 1.000 19.28 PRO 182 2301 3071 1952 -199 -245 1 MOTA ANISOU 1289 CB -199 -245 1001 1290 CG MOTA57.627 1.000 14.90 ANISOU 1290 CG 182 9.541 6.571 -421 -262 3 4 0 PRO 1291 C 1772 ATOM 1658 182 2230 57.249 1.000 15.38 PRO ANISOU 1291 C 182 8.920 5.573 -467 -482 5 3 9 183 9.969 183 1737 PRO 1292 0 1957 ATOM7.460 56.730 1.000 12.28 PRO ANISOU 1292 O 1617 -154 -284 1 5 6 HIS 1293 N MOTA 1312 7.354 55.300 1.000 11.90 1495 1614 -254 -351 3 ANISOU 1293 N HIS ANISOU 1294 CA HIS 183 1413 1495 1614 -254 -351 3 5 ATOM 1295 CB HIS 183 8.300 7.824 54.922 1.000 12.43 1 ANISOU 1295 CB HIS 183 1399 1368 1957 -128 -241 1 1 ANISOU 1296 CG HIS 183 8.168 9.314 55.089 1.000 11.36 ATOM 1296 CG HIS 183 1349 1369 1600 -367 -296 5 6 ANISOU 1297 CD2 HIS 183 8.259 10.374 54.249 1.000 12.03 ATOM 1297 CD2 HIS 183 1684 1296 1589 -43 157 -1 ANISOU 1298 ND1 HIS 183 7.989 9.858 56.339 1.000 13.27 ATOM 1298 ND1 HIS 183 1901 1439 1700 -65 267 1 9 ANISOU 1299 CE1 HIS 183 1901 1439 1700 -65 267 1 9 ANISOU 1299 CE1 HIS 183 1939 1490 1296 77 -244 150 ANISOU 1300 NE2 HIS 183 8.101 11.515 54.992 1.000 11.04 ATOM 1300 NE2 HIS 183 1560 1437 1199 215 -232 4 ANISOU 1301 C HIS 183 10.749 8.176 54.515 1.000 12.27 ANISOU 1301 C HIS 183 1446 1639 1577 -303 -282 -6 183 9.733 -254 -351 3 5 1294 CA HIS MOTA ANISOU 1294 CA HIS -128 -241 1 1 2 MOTA ANISOU 1295 CB 1600 -367 -296 5 6 MOTA -43 157 -10 267 193 77 -244 150 -232 4 8 HIS 183 10.749 8.170 34.313 1.003 282 - 6
HIS 183 1446 1639 1577 -303 -282 - 6
HIS 183 11.433 9.032 55.064 1.000 12.94
HIS 183 1496 1915 1505 -558 -292 1
HIS 184 10.849 7.907 53.215 1.000 10.61
TYR 184 1453 1027 1552 -41 -380 1 -303 -282 - 67 ANISOU 1301 C -558 -292 1 5 1302 0 MOTA ANISOU 1302 O -41 -380 1 1 0 184 10.849 184 1453 1027 1552 1000 11.36 184 11.483 104 1738 1000 11.79 1303 N MOTA ANISOU 1303 N TYR -71 -264 1 7 8 TYR 1304 CA 184 1475 1104 184 12.628 8.151 MOTA 51.481 1.000 11.79 TYR ANISOU 1304 CA 184 1631 1114 1734 -62 -197 3 4 184 12.368 6.907 50.677 1.000 11.29 184 1680 921 1688 225 -893 1 7 4 TYR 1305 CB MOTA ANISOU 1305 CB TYR TYR 1306 CG 184 12.156 5.659 51.268 1.000 11.76 184 1663 927 1879 388 -487 190 \mathtt{TYR} ANISOU 1306 CG 1307 CD1 TYR MOTA 1308 CE1 TYR 184 11.911 4.526 50.492 1.000 12.64 ANISOU 1307 CD1 TYR ATOM 1308 CE1 TYR 184 11.911 4.526 50.492 1.000 12.64

ANISOU 1308 CE1 TYR 184 1960 878 1964 173 -40 1 8 2

ATOM 1309 CD2 TYR 184 12.333 6.949 49.279 1.000 11.13

ANISOU 1309 CD2 TYR 184 1252 1302 1674 109 -283 9

ATOM 1310 CE2 TYR 184 12.102 5.834 48.502 1.000 12.93

ANISOU 1310 CE2 TYR 184 1944 1422 1546 49 -384 7 3

ANISOU 1311 CZ TYR 184 11.898 4.611 49.121 1.000 13.14

ATOM 1311 CZ TYR 184 1717 1304 1972 30 -611 6 7 TYR 184 1717 1304 TYR 184 11.663 3.490 48.343 1.000 15.45 ANISOU 1311 CZ 1312 OH MOTA

- 133 -42 - 476 - 247 2373 1471 TYR 184 2028 184 10.447 9.390 51.314 1.000 11.50 ANISOU 1312 OH -187 -201 3 4 8 TYR 1313 C 1709 1215 51.089 1.000 11.75 184 1445 TYR ANISOU 1313 C 8.797 184 9.362 -106 -171 4 2 7 TYR1314 0 1853 MOTA 1308 185 10.784 10.557 50.743 1.000 10.79 184 1305 TYRANISOU 1314 O -141 -132 1 1 8 ASP 1315 N 1449 MOTA 1069 185 1581 11.218 49.815 1.000 9.10 ANISOU 1315 N ASP 185 9.861 -326 23 2 0 6 ASP 1316 CA 1277 ATOM 1093 185 1089 12.743 49.886 1.000 10.13 ASP ANISOU 1316 CA 185 9.934 -298 -178 1 7 7 1317 CB ASP 1327 ATOM 185 1427 1095 13.388 51.185 1.000 11.79 ANISOU 1317 CB ASP 185 9.540 -250 -149 1 1 ASP 1318 CG 1333 1350 MOTA 185 1797 14.638 51.278 1.000 13.79 ASP ANISOU 1318 CG 185 9.681 -52 - 26 1319 OD1 ASP 1875 135 ATOM 1316 ANISOU 1319 OD1 ASP 185 2050 12.755 52.189 1.000 13.31 185 9.114 -411 -63 105 1320 OD2 ASP 1405 185 1805 1848 1405 -411 -03 1 185 10.098 10.759 48.371 1.000 9.44 185 1036 1150 1401 -309 -26 1 185 1036 48 005 1.000 10.6 MOTA 1848 ANISOU 1320 OD2 ASP -309 -26 100 1321 C ASP MOTA 185 11.234 10.469 48.005 1.000 10.64 ASP ANISOU 1321 C -127 -35 -206 ASP 1322 0 1500 MOTA 1376 10.684 47.568 1.000 10.09 185 1167 ASP ANISOU 1322 O 186 9.038 -272 -177 - 58 LEU 1323 N 1437 MOTA 1186 186 1211 10.312 46.161 1.000 10.60 LEU ANISOU 1323 N 186 9.124 -239 -52 -44 1324 CA LEU 986 1401 MOTA 186 1641 9.295 45.798 1.000 11.32 ANISOU 1324 CA LEU 186 8.030 929 1721 -111 17 -479 7.977 46.602 1.000 12.60 LEU 1325 CB \mathtt{MOTA} 186 1652 186 7.989 ANISOU 1325 CB LEU -263 -200 - 166 1326 CG LEU 2340 MOTA 186 1408 1039 46.028 1.000 16.64 ANISOU 1326 CG LEU 186 6.896 7.064 -634 -398 -135 1327 CD1 LEU ATOM 1373 3049 186 1900 46.629 1.000 13.84 ANISOU 1327 CD1 LEU 186 9.356 7.332 -155 443 283 1328 CD2 LEU 2575 11.521 45.223 1.000 10.90 MOTA 186 1438 ANISOU 1328 CD2 LEU 186 9.024 -3 -451 164 LEU 1329 C 1603 MOTA 1211 11.406 44.031 1.000 13.60 186 1327 ANISOU 1329 C LEU 186 8.768 -321 1 0 3 LEU 1330 0 -211 ATOM 1494 1608 186 2067 12.705 45.734 1.000 10.71 ANISOU 1330 O LEU SER 187 9.264 -282 3 1 8 1331 N -76 1393 MOTA 1129 13.943 44.998 1.000 10.49 SER 187 1546 ANISOU 1331 N SER 187 9.401 -107 4 8 8 1332 CA 195 1370 MOTA 1191 187 1427 15.103 46.002 1.000 10.56 ANISOU 1332 CA SER 187 9.221 187 1105 161 532 SER 298 1333 CB 1857 MOTA 1048 187 10.430 14.918 46.726 1.000 13.01 SER ANISOU 1333 CB -132 -295 2 0 1 SER 2169 1334 OG MOTA 187 1343 1432 187 10.774 14.062 44.336 1.000 10.47 ANISOU 1334 OG SER 862 1669 135 -3 1 4 5 SER 1335 C MOTA 187 1447 187 11.684 13.246 44.513 1.000 10.54 SER ANISOU 1335 C 183 -91 - 77 1336 0 SER 799 1629 MOTA 15.095 43.502 1.000 9.78 187 1577 SER ANISOU 1336 O 188 10.962 978 1318 147 44 7 4 1337 N MET MOTA 188 12.267 15.584 43.065 1.000 9.94 188 1419 MET ANISOU 1337 N 182 58 3 7 MET 1338 CA 942 1441 MOTA 188 12.128 16.543 41.891 1.000 10.89 188 1394 MET ANISOU 1338 CA 98 48 2 2 7 1339 CB MET 840 1774 MOTA 188 1523 188 13.385 17.258 41.470 1.000 11.40 ANISOU 1339 CB MET 46 -51 214 MET 1340 CG 1756 MOTA 1172 188 1403 188 14.687 16.134 40.891 1.000 12.71 MET ANISOU 1340 CG 137 198 MET 1341 SD 139 1940 MOTA 1272 188 16.061 17.267 40.790 1.000 13.86 188 1619 MET ANISOU 1341 SD -2 911 - 90 MET 1342 CE ATOM 2003 1399 188 1862 ANISOU 1342 CE MET

- 134 -188 12.946 16.217 44.291 1.000 12.13 169 -18 -285 MET 1343 C 1698 MOTA 1586 188 13.971 15.727 44.804 1.000 11.52 ANISOU 1343 C MET 144 132 8 7 MET 1344 0 1535 1553 VAL 189 12.362 17.290 44.838 1.000 10.00 188 1288 ANISOU 1344 O 1345 N 1217 1292 1346 CA VAL 189 12.745 17.894 46.099 1.000 9.70 ANISOU 1345 N VAL 189 1209 1057 1420 -212 -45 -VAL 189 13.618 19.154 45.979 1.000 9.97 -212 -45 -19 MOTA ANISOU 1346 CA ATOM 1347 CB VAL 105 13.010 19.134 43.575 1.000 9.57 ANISOU 1348 CG1 VAL 189 14.953 18.837 45.266 1.000 13.45 ATOM 1348 CG1 VAL 189 1334 1410 2368 -236 390 1 4 3 ANISOU 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ATOM 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ANISOU 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ANISOU 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ANISOU 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24 ATOM 1349 CG2 VAL 189 12.899 20.289 45.264 1.000 12.24
ANISOU 1349 CG2 VAL 189 1715 1242 1693 -25 150 25
ATOM 1350 C VAL 189 11.469 18.245 46.871 1.000 10.10
ATOM 1350 C VAL 189 10.89 1600 1149 -456 -156 ANISOU 1351 O VAL 189 10.405 18.399 46.250 1.000 9.53
ATOM 1351 O VAL 189 1153 1249 1217 -222 -190 8
ANISOU 1352 N THR 190 11.609 18.327 48.187 1.000 8.666
ATOM 1352 N THR 190 1273 894 1123 15 -202 127 -156 - 73 THR 190 1273 894 1123 15 -202 127 190 10.565 18.771 49.091 1.000 9.64 190 1350 1167 1147 -11 -228 -ANISOU 1352 N -11 -228 - 9 9 1353 CA THR MOTA 190 10.194 17.699 50.132 1.000 10.69 ANISOU 1353 CA THR -300 121 -54 THR 1354 CB 190 1231 1196 1635 MOTA 190 9.662 16.586 49.501 1.000 12.45 ANISOU 1354 CB THR -140 -258 - 48 1355 OG1 THR 190 1333 1341 190 9.038 18.131 2055 MOTA18.131 51.019 1.000 13.59 ANISOU 1355 OG1 THR 1821 -272 151 -195 1356 CG2 THR THR 190 11.058 19.976 49.891 1.000 9.23 THR 190 1257 1096 1152 -102 -336 -MOTA ANISOU 1356 CG2 THR 1096 1152 -102 -336 - 49 1357 C ATOMTHR 190 12.149 19.867 50.447 1.000 10.54 ATOM 1358 O THR 190 12.149 19.867 50.447 1.000 10.54

ANISOU 1358 O THR 190 1322 1292 1390 -5 -359 -122

ATOM 1359 N LEU 191 10.313 21.064 49.978 1.000 10.23

ANISOU 1359 N LEU 191 1319 1167 1401 -71 -177 -133

ANISOU 1360 CA LEU 191 10.691 22.241 50.770 1.000 10.19

ANISOU 1360 CA LEU 191 1259 1176 1438 0 -294 -142

ANISOU 1361 CB LEU 191 10.604 23.511 49.910 1.000 11.52

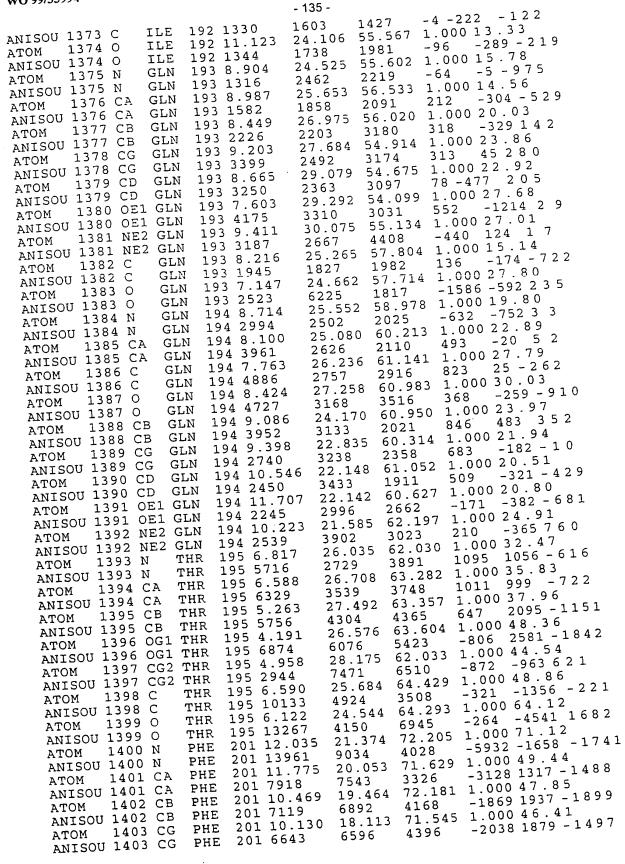
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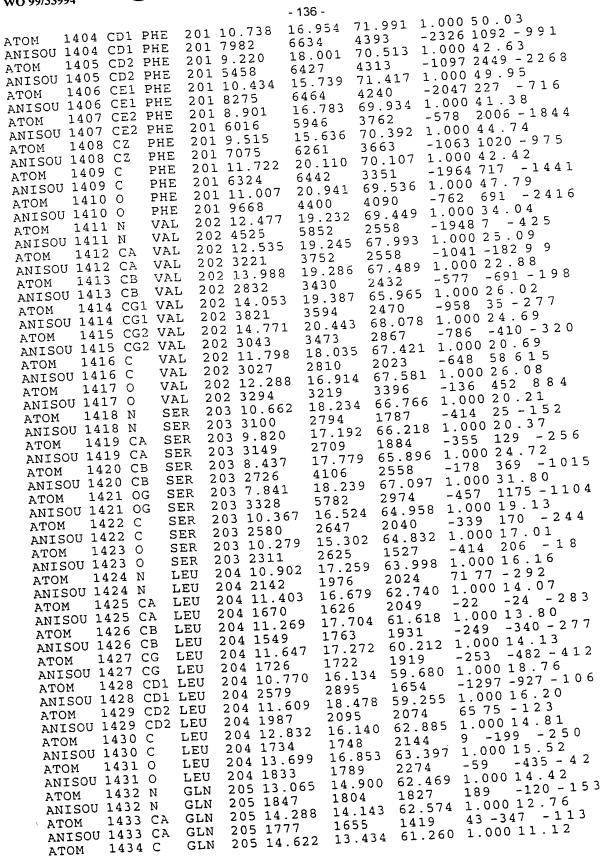
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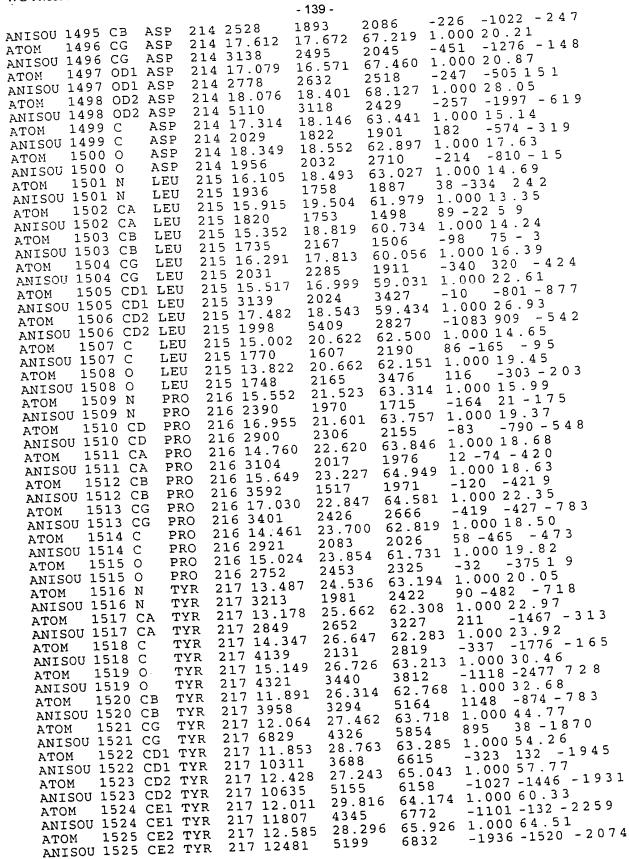
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- 137 -49 - 468 - 21 1338 1474 205 13.707 12.927 60.606 1.000 13.97 205 1412 GLN ANISOU 1434 C -293 -449 -147 1435 0 GLN1449 ATOM 2235 205 14.164 13.062 63.662 1.000 15.57 ANISOU 1435 O GLN341 151 8 3 GLN 1436 CB 1568 1925 205 13.863 13.635 65.032 1.000 18.58 205 2421 GLN ANISOU 1436 CB 689 -129 8 2 1437 CG GLN1451 MOTA 2286 205 15.086 14.243 65.680 1.000 24.33 ANISOU 1437 CG GLN 520 -499 - 570 1438 CD GLN2091 MOTA 3465 205 3687 3465 2091 320 205 16.206 13.717 65.549 1.000 29.12 ANISOU 1438 CD GLN14 -270 -1800 1439 OE1 GLN ATOM4251 205 3350 3464 205 14.840 15.356 66.378 1.000 23.01 ANISOU 1439 OE1 GLN 1440 NE2 GLN -592 - 140 335 3225 MOTA 205 3055 2465 ANISOU 1440 NE2 GLN 206 15.893 13.401 60.893 1.000 12.63 -251 -234 - 6 ALA 1441 N 1506 ATOM 1770 206 16.335 12.649 59.731 1.000 13.77 206 1523 ALAANISOU 1441 N -522 -72 -295 ALA1442 CA 1742 MOTA 206 16.693 13.519 58.528 1.000 16.34 ALA 206 1392 ANISOU 1442 CA -603 123 -277 ALA1443 CB 1682 2494 MOTA 206 17.567 11.813 60.046 1.000 15.92 206 2034 ANISOU 1443 CB ALA -290 179 -341 206 1489 2331 2230 -290 179 -3 206 18.368 12.182 60.908 1.000 15.86 1444 C ALAATOM ALA ANISOU 1444 C 150 -356 3 0 1445 0 ALA2377 MOTA 1772 206 1877 207 17.707 10.712 59.305 1.000 16.98 ALA ANISOU 1445 O -335 348 -186 GLU 1446 N 2383 ATOM2086 59.364 1.000 20.58 207 1981 ANISOU 1446 N GLU 207 18.938 9.942 -164 490 -10 ${ t GLU}$ 1447 CA 3684 ATOM207 20.082 10.688 58.681 1.000 18.75 ANISOU 1447 CA GLU 272 185 558 GLU 1448 C MOTA 2037 3260 GLU 207 19.948 10.953 57.503 1.000 18.23 ANISOU 1448 C 1449 0 3034 ATOM 2145 207 1746 58.676 1.000 25.81 ANISOU 1449 O GLU 207 18.665 8.612 83 - 135 1450 CB GLU -19 GLU 207 3289 1794 GLU 207 19.879 7.737 4724 MOTA1794 58.429 1.000 30.08 ANISOU 1450 CB -948 - 546 907 1451 CG 5105 ATOM 2221 207 4102 57.959 1.000 29.93 ANISOU 1451 CG ${ t GLU}$ 207 19.429 6.356 1179 -2099 -123 GLU 1452 CD 3798 207 5549 2024 207 19.491 5.471 MOTA58.839 1.000 35.14 ANISOU 1452 CD GLU -931 8 8 5 1453 OE1 GLU 938 4879 MOTA 2692 56.762 1.000 38.62 207 5782 ANISOU 1453 OE1 GLU 207 19.037 6.251 -2494 - 366 1454 OE2 GLU 135 4109 MOTA VAL 208 21.146 10.997 59.414 1.000 16.97 5608 ANISOU 1454 OE2 GLU 337 807 1455 N 1974 MOTA VAL 208 22.376 11.593 58.902 1.000 17.77 ANISOU 1455 N 1456 CA MOTA 2109 208 22.455 13.111 59.155 1.000 16.89 VAL 208 1894 ANISOU 1456 CA -372 -149 5 6 9 VAL 1457 CB 1494 ATOM 2148 208 2774 208 23.652 13.688 58.409 1.000 20.76 ANISOU 1457 CB VAL -423 647 148 1458 CG1 VAL MOTA 2526 2150 208 3214 208 21.172 13.815 58.720 1.000 16.36 ANISOU 1458 CG1 VAL 25 98 3 5 3 1459 CG2 VAL MOTA 1431 208 23.585 10.877 59.507 1.000 20.29 ANISOU 1459 CG2 VAL VAL 208 1936 2555 3217 11 -58 1 3 2 VAL 208 23.726 10.829 60.741 1.000 20.74 1460 C MOTA ANISOU 1460 C 206 544 1461 0 3187 MOTA 2256 GLY 209 24.457 10.295 58.672 1.000 18.94 ANISOU 1461 O -494 1 5 1462 N 2989 MOTA GLY 209 1764 2445 59.194 1.000 24.01 ANISOU 1462 N 209 25.558 9.508 -396 7 0 9 1463 CA GLY549 MOTA 3910 3040 60.082 1.000 25.00 209 2171 GLYANISOU 1463 CA 8.364 209 25.123 1406 772 649 GLY 1464 C 3470 MOTA 3156 209 2874 GLY ANISOU 1464 C

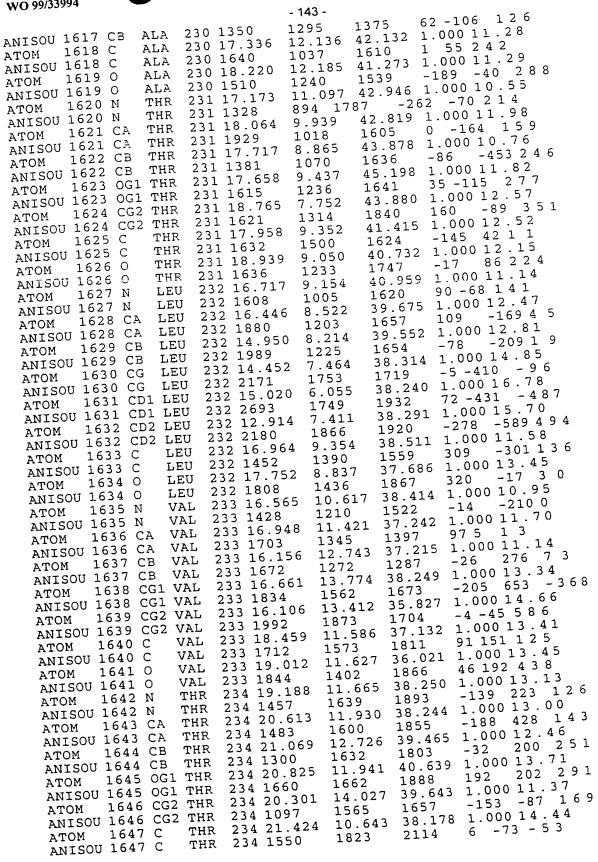
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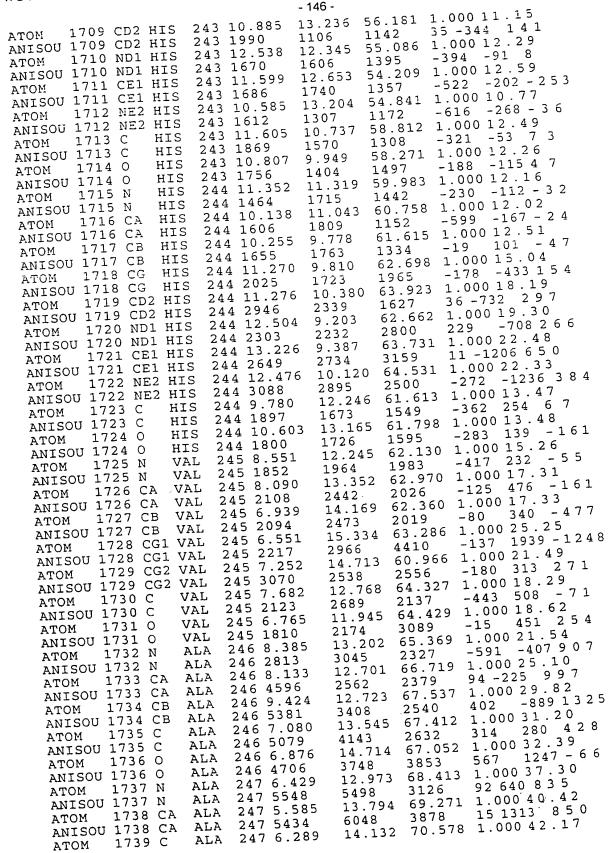
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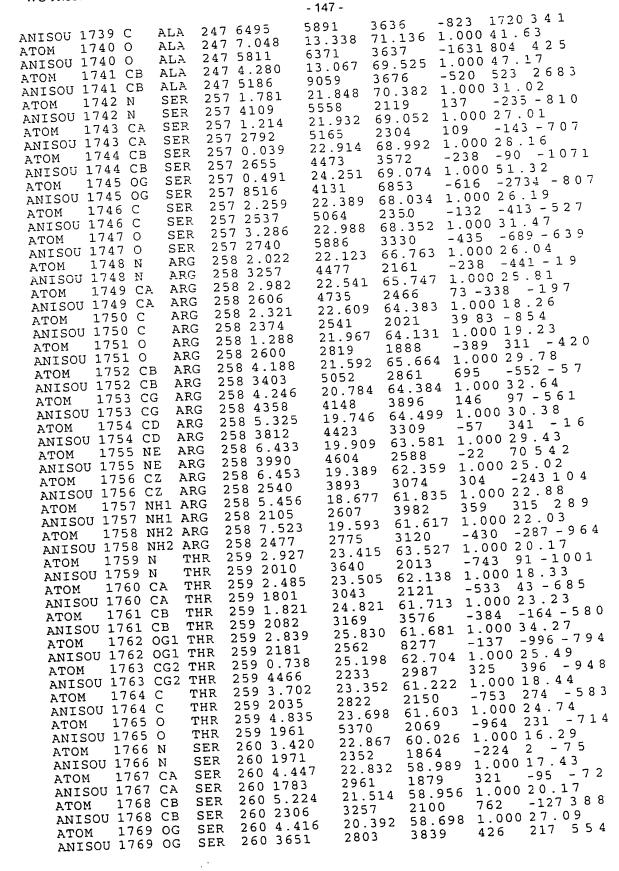
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- 144 -THR 234 22.659 10.710 38.233 1.000 15.81 1648 0 2169 2293 ATOM 38.070 1.000 14.76 234 1546 THR ANISOU 1648 O 235 20.767 9.477 77 81 410 GLY 1649 N 2254 1576 235 1776 37.994 1.000 16.69 GLYANISOU 1649 N 235 21.530 8.249 35 1 8 9 1650 CA GLY304 2486 ATOM 235 2053 1803 235 22.243 7.862 39.275 1.000 16.83 ANISOU 1650 CA GLY244 193 GLY765 1651 C 2512 MOTA 2031 39.194 1.000 19.67 235 1854 GLY ANISOU 1651 C 235 23.305 7.237 1035 383 372 GLY1652 0 235 2074 2172 3225 1035 383 3 236 21.665 8.227 40.425 1.000 14.46 3225 MOTA ANISOU 1652 O GLY 198 7 236 1732 1327 2433 154 198 7 236 22.187 7.768 41.692 1.000 15.73 236 2060 1381 2536 41 186 3 1 2 GLY 1653 N MOTA GLYANISOU 1653 N GLY1654 CA ATOM 236 23.166 8.691 42.388 1.000 14.76 GLYANISOU 1654 CA 73 2 8 8 GLY252 1655 C 236 1931 1332 2346 MOTA 236 23.778 8.244 43.373 1.000 18.32 GLY ANISOU 1655 C 236 1983 2197 2782 106 -105 8 4 237 23.318 9.938 41.953 1.000 13.99 -105 8 4 4 1656 0 GLYMOTA ANISOU 1656 O GLY237 1831 1349 2137 158 165 1 237 24.209 10.956 42.485 1.000 13.13 158 165 170 GLN1657 N MOTA GLN ANISOU 1657 N 367 -31 276 1658 CA GLN 2210 MOTA 1304 237 24.629 11.948 41.383 1.000 13.38 GLNANISOU 1658 CA 1659 CB GLN2151 MOTA 1566 237 25.390 11.335 40.219 1.000 14.74 ANISOU 1659 CB GLN410 333 GLN1660 CG 2666 MOTA 237 25.816 12.428 39.257 1.000 17.22 1529 ANISOU 1660 CG GLN426 360 GLN 1661 CD 2486 ATOM2018 1662 OE1 GLN 237 26.754 13.208 39.522 1.000 20.60 ANISOU 1661 CD ANISOU 1662 OE1 GLN 237 1566 2334 3928 -10 -29 9
ANOM 1663 NE2 GLN 237 25.116 12.470 38.127 1.000 17.47 -29 965 208 438 408 237 23.627 11.739 43.663 1.000 12.90 ANISOU 1663 NE2 GLN ATOM 1664 C GLN 237 2014 2104 1324 GLN 237 24.332 12.549 44.282 1.000 15.90 ANISOU 1664 C -291 74 - 84 1665 0 VAL 238 22.365 11.481 44.013 1.000 12.13 ATOM ANISOU 1665 O 962 2276 212 1666 N MOTAVAL 238 21.664 12.182 45.082 1.000 11.91 ANISOU 1666 N -121 -276 - 19 1667 CA MOTA 1436 VAL 238 1169 VAL 238 20.622 13.158 44.510 1.000 12.00 ANISOU 1667 CA 1668 CB 1179 MOTA 238 1024 238 19.978 13.999 45.601 1.000 13.07 VAL ANISOU 1668 CB 63 -232 - 222 1669 CG1 VAL 1767 MOTA 1668 238 21.207 14.088 43.463 1.000 14.00 ANISOU 1669 CG1 VAL -40 -2 1 8 1 1670 CG2 VAL 2053 MOTA 1470 238 20.990 11.156 46.000 1.000 13.62 238 1795 ANISOU 1670 CG2 VAL -103 -40 -22 VAL 1671 C 2054 MOTA 1415 VAL 238 1707 VAL 238 20.252 10.288 45.492 1.000 12.64 ANISOU 1671 C 977 2123 60 -318 257 1672 0 MOTA LYS 239 21.247 11.246 47.300 1.000 11.99 ANISOU 1672 O -101 7 4 1673 N MOTA 1404 239 20.568 10.444 48.322 1.000 12.77 ANISOU 1673 N LYS -124 8 6 1674 CA LYS 1541 2088 MOTA 239 1224 239 21.382 10.463 49.622 1.000 12.23 ANISOU 1674 CA LYS -234 - 28 1675 CB LYS 2158 ATOM 1155 50.793 1.000 13.85 239 1333 ANISOU 1675 CB LYS 239 20.953 9.626 -52 - 89 LYS 187 1676 CG MOTA 1931 1689 239 1643 51.957 1.000 20.13 LYS ANISOU 1676 CG 239 21.927 9.579 10 -1185 588 1677 CD LYS MOTA 2961 1795 53.098 1.000 24.73 239 2893 LYS ANISOU 1677 CD 239 21.364 8.745 1678 CE LYS MOTA

- 145 --348 -1465 1064 3080 2250 54.420 1.000 32.28 239 4065 ANISOU 1678 CE LYS 8.841 239 22.019 1610 -930 - 304 1679 NZ LYS 2293 MOTA 4315 10.949 48.661 1.000 11.59 239 5658 ANISOU 1679 NZ LYS 239 19.169 -35 -82 6 LYS 1680 C 1866 MOTA 1332 48.708 1.000 12.32 239 1207 ANISOU 1680 C LYS 12.191 239 18.976 -2 -25 2 3 6 LYS 1681 0 1749 MOTA 1294 239 1638 48.863 1.000 10.65 ANISOU 1681 0 LYS 10.047 240 18.222 1682 N ALA -185 - 88 -52 1534 MOTA 1266 ALA 240 1248 10.368 49.354 1.000 10.21 ANISOU 1682 N ALA 240 16.884 10.368 ALA 240 1292 1057 ALA 240 15.784 9.782 ALA 240 1195 2378 ALA 240 16.784 9.881 -195 -37 -109 1683 CA 1531 ATOM 48.466 1.000 13.46 ANISOU 1683 CA -232 20 -403 1684 CB 1543 MOTA 50.807 1.000 10.97 ANISOU 1684 CB -127 -142 4 9 1685 C 1611 MOTA ALA 240 1308 1249 51.059 1.000 13.02 ANISOU 1685 C ALA 240 16.595 8.664 28 - 71686 O -243 MOTA 1568 ALA 240 2136 241 16.967 10.783 51.782 1.000 11.13 1242 ANISOU 1686 O -49 138 PRO 1687 N 160 1466 ATOM 1041 241 17.172 12.237 51.654 1.000 11.17 241 1723 ANISOU 1687 N PRO -180 -128 7 6 1688 CD PRO MOTA PRO ANISOU 1688 CD -172 -32 193 1689 CA PRO 1499 MOTA 1447 241 1597 11.545 53.891 1.000 14.25 PRO ANISOU 1689 CA 241 17.712 -531 -383 2 4 2 PRO 1690 CB 1701 1837 MOTA 241 1875 241 17.286 12.724 53.069 1.000 13.61 ANISOU 1690 CB PRO -596 -465 - 22 1691 CG PRO 1709 MOTA 1446 53.861 1.000 12.35 241 2015 ANISOU 1691 CG PRO 241 15.708 10.072 -175 -187 4 1 8 PRO 1692 C ATOM 1665 1610 241 1417 53.655 1.000 12.28 PRO ANISOU 1692 C 10.829 241 14.759 -232 -468 8 1 PRO 1693 0 MOTA 1582 241 1359 ANISOU 1693 O PRO 9.033 242 15.700 -170 76 2 5 0 1694 N ARG 1664 MOTA 1407 55.576 1.000 10.76 242 1775 ARG ANISOU 1694 N 8.804 242 14.563 -207 -281 2 1 1 ARG 1695 CA MOTA 1417 1380 242 1292 56.223 1.000 15.02 ANISOU 1695 CA ARG 7.405 242 14.614 -357 117 294 ARG 1696 CB 1918 MOTA 1368 242 2419 55.230 1.000 17.85 ANISOU 1696 CB ARG 242 14.115 6.342 9 -560 251 1697 CG ARG 2135 MOTA 1274 55.763 1.000 19.42 242 3373 ANISOU 1697 CG ARG 242 14.254 4.934 503 116 ARG 1698 CD 506 3120 ATOM 1111 55.849 1.000 20.71 242 3148 ARG ANISOU 1698 CD 242 15.667 4.552 638 212 1699 NE ARG 938 2538 MOTA 2107 242 3225 56.416 1.000 23.22 ANISOU 1699 NE ARG 242 16.107 3.444 -544 5 8 9 1700 CZ ARG 307 3417 MOTA 2206 242 3198 56.980 1.000 24.46 ANISOU 1700 CZ ARG 242 15.285 2.567 387 195 1701 NH1 ARG 307 MOTA 3083 2112 56.438 1.000 25.41 242 4097 ANISOU 1701 NH1 ARG 242 17.416 3.184 819 -267 4 0 3 1702 NH2 ARG MOTA 2332 3921 242 3402 56.704 1.000 11.95 ANISOU 1702 NH2 ARG 242 14.477 9.834 -248 -214 1 0 7 1703 C ARG 1506 MOTA 1463 242 1571 57.213 1.000 13.65 ANISOU 1703 C ARG 242 15.469 10.377 -322 -401 - 38 ARG 1704 0 2040 MOTA 1439 242 1708 57.118 1.000 11.60 ARG ANISOU 1704 O 243 13.252 10.085 -311 -206 5 HIS 1705 N MOTA 1342 1410 243 12.942 11.056 58.158 1.000 11.49 ANISOU 1705 N HIS 938 -306 -183 140 1706 CA HIS MOTA 1571 12.462 57.546 1.000 11.22 243 1855 ANISOU 1706 CA HIS 243 12.968 -231 -221 3 9 HIS 1707 CB MOTA 1453 1379 243 1432 56.341 1.000 11.80 HIS ANISOU 1707 CB 12.694 243 12.133 -268 7 9 HIS 1708 CG -31 1378 MOTA 1171 243 1937 HIS ANISOU 1708 CG





- 148 -23.062 57.614 1.000 14.52 SER 260 3.832 1770 C 83 -100 - 1 1889 MOTA 2165 260 1463 22.681 57.402 1.000 15.92 SER ANISOU 1770 C 260 2.686 SER -93 -1 2 5 7 1771 0 ATOM 2049 2489 23.660 56.742 1.000 13.45 260 1513 ANISOU 1771 O SER 261 4.617 -190 -120 -500 SER 1772 N MOTA 1788 1832 261 1489 23.864 55.334 1.000 13.52 ANISOU 1772 N SER 261 4.294 1773 CA SER -204 30 -315 ATOM 1812 1726 261 1599 22.943 54.545 1.000 12.45 ANISOU 1773 CA SER 261 5.209 -240 - 161 1774 C SER -42 ATOM 1513 1887 261 1332 23.072 54.662 1.000 15.07 ANISOU 1774 C SER 261 6.438 SER 1775 0 -331 -343 -68 ATOM 2497 1885 261 1344 25.330 54.943 1.000 17.76 SER ANISOU 1775 O 261 4.446 1776 CB SER -399 -485 -318 2404 MOTA 1625 261 2718 25.554 53.570 1.000 27.54 ANISOU 1776 CB SER 261 4.428 -719 -821 955 1777 OG SER MOTA 2814 3308 262 4.623 22.045 53.782 1.000 10.90 261 4342 ANISOU 1777 OG SER 41 -135 1 9 1778 N VAL 262 1215 1630 1299 41 -135 1 9 262 5.393 21.031 53.026 1.000 11.61 ATOM ANISOU 1778 N VAL 156 -103 1 7 1779 CA VAL MOTA 1442 1634 262 1334 19.639 53.558 1.000 11.87 ANISOU 1779 CA VAL 262 5.026 9 -187 - 74 VAL 1780 CB MOTA 1614 1636 262 1262 18.577 52.779 1.000 13.12 ANISOU 1780 CB VAL 262 5.778 1781 CG1 VAL -2 185 5 1 MOTA 1997 1527 262 1462 19.564 55.062 1.000 17.08 ANISOU 1781 CG1 VAL 1782 CG2 VAL 262 5.262 -374 -245 3 9 MOTA 1604 ANISOU 1782 CG2 VAL 262 3390 1494 21.149 51.543 1.000 11.18 VAL 262 5.096 1 -111 -138 1783 C ATOM 20.969 51.127 1.000 12.76 1431 VAL 262 1026 VAL 262 3.939 VAL 262 1064 PHE 263 6.090 ANISOU 1783 C -251 -84 -271 2137 1648 -251 -84 -21.438 50.714 1.000 9.50 1784 0 \mathtt{MOTA} ANISOU 1784 O 263 995 1297 1316 -6 -210 -181 1785 N ATOM263 5.933 21.637 49.288 1.000 9.61 PHE ANISOU 1785 N -6 -284 - 42 PHE 1786 CA MOTA 1324 1017 263 1310 23.002 48.848 1.000 10.94 ANISOU 1786 CA PHE 263 6.486 -253 4 1787 CB PHE 263 1282 1055 1821 -50 -253 4 263 6.150 23.399 47.418 1.000 10.35 MOTA ANISOU 1787 CB PHE PHE 263 779 1231 1921 -58 1788 CG MOTA 263 6.858 22.915 46.326 1.000 9.98 ANISOU 1788 CG PHE 263 766 1183 1841 -26 -101 240 1789 CD1 PHE MOTA 263 5.106 24.277 47.148 1.000 11.95 263 1229 1261 2052 245 -29 2 ANISOU 1789 CD1 PHE -29 261 1790 CD2 PHE MOTA 263 6.530 23.229 45.019 1.000 12.49 ANISOU 1790 CD2 PHE 31 - 370 136 1791 CE1 PHE MOTA 1857 1173 263 4.769 24.601 45.836 1.000 13.12 263 1718 ANISOU 1791 CE1 PHE 43 - 292 353 1792 CE2 PHE MOTA 1382 2151 263 1451 263 5.491 24.112 44.762 1.000 12.42 ANISOU 1792 CE2 PHE -138 -187 6 4 9 1793 CZ PHE 1948 263 1318 263 6.636 20.505 1076 1085 1453 263 1318 20.505 48.530 1.000 8.91 PHE ANISOU 1793 CZ -39 -142 2 4 PHE 1794 C 1223 MOTA 20.406 48.538 1.000 10.98 ANISOU 1794 C PHE 263 7.868 -120 -224 - 145 1795 0 PHE MOTA 1842 1233 19.691 47.812 1.000 9.19 PHE 263 1098 ANISOU 1795 O -105 - 82 264 5.856 PHE 1796 N -86 MOTA 1136 1266 264 1089 18.602 46.991 1.000 9.64 ANISOU 1796 N PHE 264 6.386 -60 -126 PHE 1797 CA -56 1417 MOTA 1238 17.358 47.005 1.000 9.92 264 1009 ANISOU 1797 CA PHE 264 5.483 1798 CB PHE 17 9 -78 MOTA 1359 1201 264 1209 16.673 48.336 1.000 11.22 ANISOU 1798 CB PHE 264 5.265 PHE 1799 CG -121 1374 MOTA 1647 264 1241 16.236 49.139 1.000 15.38 ANISOU 1799 CG PHE 264 6.292 1800 CD1 PHE MOTA

- 149 --225 -8873 1734 2641 ANISOU 1800 CD1 PHE 264 1467 16.433 48.808 1.000 16.96 264 3.988 -610 -79 958 1801 CD2 PHE 264 1425 1769 3252 ANISOU 1801 CD2 PHE 15.596 50.336 1.000 14.52 264 6.090 1802 CE1 PHE 334 452 162 MOTA 1354 2417 264 1745 ANISOU 1802 CE1 PHE 264 3.755 15.796 50.019 1.000 18.04 264 1747 3405 1704 -590 -109 10 264 4.817 15.354 50.779 1.000 12.52 264 1772 1536 1449 -57 227 3 264 6.535 19.038 45.533 1.000 8.98 264 1103 919 1392 143 81 -92 264 5.497 19.368 44.930 1.000 9.79 264 991 1190 1540 28 105 103 1803 CE2 PHE -590 -109 1008 ATOM ANISOU 1803 CE2 PHE PHE 1804 CZ ANISOU 1804 CZ PHE PHE 1805 C ATOM PHE ANISOU 1805 C 1806 0 PHE 264 991 1190 1540 28 105 1 0 3 LEU 265 7.758 19.031 44.999 1.000 8.43 PHE ATOM ANISOU 1806 O 265 992 884 1325 173 -180 158 265 7.984 19.224 43.566 1.000 8.66 1807 N MOTA LEU ANISOU 1807 N 1808 CA LEU 265 883 1066 1339 63 -33 MOTA ANISOU 1808 CA LEU 265 9.309 19.964 43.328 1.000 10.10 ren ----225 -220 2 4 8 1809 CB MOTA 1188 1469 265 9.570 20.351 41.871 1.000 9.37 265 1179 ANISOU 1809 CB LEU 242 25 1 2 9 1810 CG LEU ATOM 1478 1009 LEU 265 1072 21.522 41.408 1.000 10.80 1810 CG LEU 265 1072 1811 CD1 LEU 265 8.725 ANISOU 1810 CG 1811 181 -114 2 9 6 ATOMANISOU 1811 CD1 LEU 265 1291 1004 1812 CD2 LEU 265 11.048 20.684 41.678 1.000 10.87 ATOM 1812 CD2 LEU 265 1129 1483 1519 134 43 146

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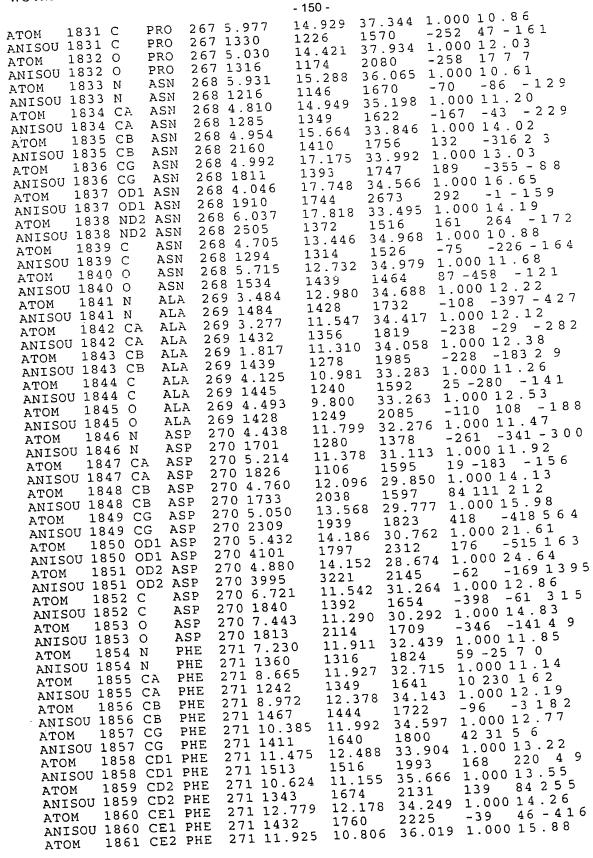
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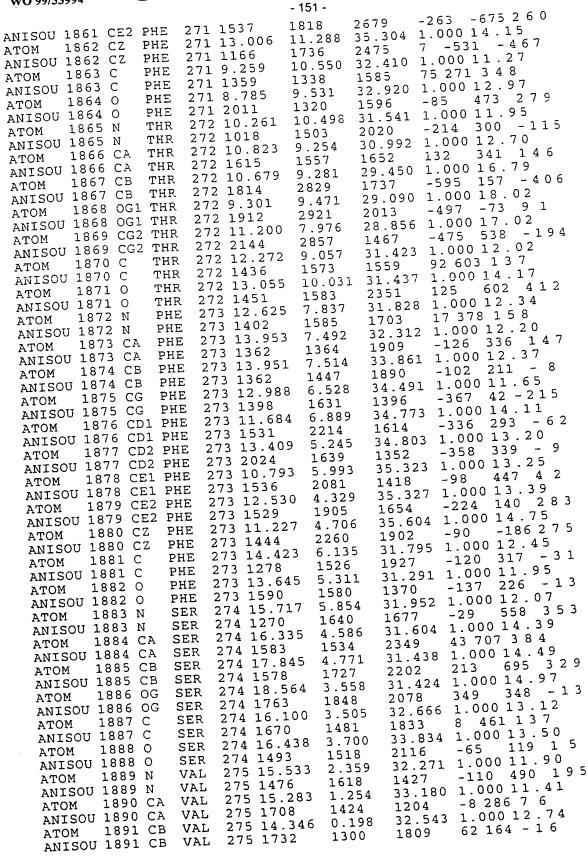
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ARG 266 1113 1567 1564 -17 -49
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ARG 266 1341 1157 1086 24 -100 -14 1817 CB ARG MOTAANISOU 1817 CB 119 206 1818 CG ATOM ANISOU 1818 CG -49 -11 1819 CD MOTA ANISOU 1819 CD 266 1341 1157 1086 24 -100 -1 266 1.236 15.509 43.657 1.000 9.83 24 -100 -145 1820 NE ARG MOTA ANISOU 1820 NE 132 -159 - 1 1821 CZ ARG MOTA 266 1245 1194 1294 266 0.961 14.567 44.572 1.000 11.20 ANISOU 1821 CZ ARG 1822 NH1 ARG 266 1208 1240 1806 1823 NH2 ARG 266 0.225 16.048 42.975 1823 NH2 ARG 266 1460 1265 1484 -144 -454 2 7 2 1822 NH1 ARG 16.048 42.975 1.000 11.08 ANISOU 1822 NH1 ARG 191 -283 7 3 ATOM ANISOU 1823 NH2 ARG 266 1460 16.190 40.099 1.000 10.28 1089 1545 -200 -5 -16 ARG 266 6.601 -200 -5 -167 1824 C MOTA ARG 266 1273 17.109 39.519 1.000 11.05 ANISOU 1824 C ARG 266 6.027 ARG 266 1254 1153 1793 -132 47 - 6 4 PRO 267 7.215 15.162 39.496 1.000 10.27 -132 47 - 64 1825 0 MOTA ANISOU 1825 O 267 1194 1239 1468 -33 130 3 267 7.828 13.963 40.109 1.000 12.36 130 3 2 1826 N MOTA ANISOU 1826 N PRO 1827 CD PRO -529 - 192 ATOM 1697 PRO 267 7.304 15.157 38.036 1.000 10.12 ANISOU 1827 CD PRO -129 38 - 185 1828 CA MOTA 267 1278 1095 1472 13.986 37.767 1.000 11.83 PRO ANISOU 1828 CA 267 8.250 90 - 322 PRO 1829 CB 267 1489 1088 1919 -/2 90 -32 267 8.017 13.053 38.913 1.000 10.72 1919 -72 MOTA 267 1489 ANISOU 1829 CB PRO PRO 95 -257 -187 1830 CG MOTA 1755 267 960 1356 ANISOU 1830 CG PRO





- 152 --1.020 33.437 1.000 16.10 275 14.157 -614 -663 3 7 0 1892 CG1 VAL MOTA 1962 1803 32.261 1.000 13.81 275 2352 ANISOU 1892 CG1 VAL 0.763 275 12.961 16 363 1 2 6 1893 CG2 VAL 1924 1786 275 1535 ANISOU 1893 CG2 VAL 33.692 1.000 12.62 0.622 275 16.577 14 375 1 3 6 VAL 1894 C 1594 MOTA 1628 275 1574 34.926 1.000 13.01 ANISOU 1894 C VAL 275 16.729 0.405 VAL 275 1667 1643 276 17.569 0.286 9 118 180 1895 0 MOTA 1634 32.889 1.000 14.64 ANISOU 1895 O VAL PRO 2 454 - 42 1896 N 1914 ATOM 2066 276 1583 31.415 1.000 15.84 PRO ANISOU 1896 N 0.285 276 17.583 PRO 89 755 3 5 1897 CD 1916 ATOM 2536 276 1565 -0.250 33.453 1.000 16.76 ANISOU 1897 CD PRO 276 18.827 393 -163 1898 CA PRO 261 2296 MOTA 2403 276 1667 -0.503 32.236 1.000 18.27 ANISOU 1898 CA PRO 276 19.732 574 - 142 1899 CB PRO 411 2571 ATOM 2568 276 1804 276 18.868 -0.385 31.029 1.000 18.96 PRO ANISOU 1899 CB 694 - 37 PRO 1900 CG 2293 ATOM 2763 276 2147 34.420 1.000 16.32 ANISOU 1900 CG PRO 276 19.500 0.710 237 6 7 PRO 115 1901 C 2336 ATOM 2342 35.456 1.000 16.78 276 1521 PRO ANISOU 1901 C 276 20.035 0.277 93 376 253 PRO 1902 0 2275 ATOM 2689 276 1411 1.000 16.58 PRO ANISOU 1902 O 34.155 277 19.475 2.019 483 148 LEU -15 1903 N 2052 MOTA 2412 35.099 1.000 17.70 277 1835 ANISOU 1903 N LEU 277 20.142 2.919 362 118 1904 CA LEU -21 2511 MOTA 2226 277 1990 34.425 1.000 20.20 ANISOU 1904 CA LEU 277 20.298 4.277 -1 -14 271 LEU 1905 CB 2432 MOTA 2292 277 2952 35.186 1.000 20.86 ANISOU 1905 CB LEU 277 21.048 5.359 -355 4 8 2 LEU 1906 CG -32 3490 ATOM 2221 35.531 1.000 34.24 277 2213 ANISOU 1906 CG LEU 277 22.446 4.888 69 -842 258 1907 CD1 LEU MOTA 8552 2303 34.334 1.000 31.91 277 2157 ANISOU 1907 CD1 LEU 277 21.062 6.620 -474 -572 1150 1908 CD2 LEU 277 4745 2460 277 19.411 2.989 4918 ATOM 36.430 1.000 16.55 ANISOU 1908 CD2 LEU -218 211 -243 LEU 1909 C 2430 ATOM 1885 37.517 1.000 19.19 277 1975 277 1975 1883 277 19.997 3.116 ANISOU 1909 C LEU -617 50 1 2 2 LEU 1910 0 2476 MOTA 2636 277 2179 36.386 1.000 15.48 ANISOU 1910 O LEU ALA 278 18.080 2.905 -358 279 112 1911 N 1969 ATOM 1904 37.636 1.000 14.51 278 2008 ALA ANISOU 1911 N 278 17.308 2.896 -309 74 1 6 7 ALA 1912 CA 1641 MOTA 1763 37.347 1.000 15.41 278 2109 ALA ANISOU 1912 CA 278 15.814 2.896 66 301 6 2 6 1913 CB ALA2064 MOTA 1773 278 2017 38.479 1.000 14.55 ALA ANISOU 1913 CB 278 17.710 1.684 -195 -255 7 9 ALA 1914 C 1689 1869 MOTA 39.683 1.000 13.80 278 1972 ALA ANISOU 1914 C 278 17.894 1.770 -250 -166 8 9 ALA 1915 0 1655 MOTA 2144 37.842 1.000 13.86 278 1444 ANISOU 1915 O ALA 279 17.841 0.530 -432 -128 1 6 9 1916 N ARG 1742 MOTA -0.679 38.560 1.000 15.88 1728 279 1795 ANISOU 1916 N ARG 279 18.242 59 355 4 1 1 ARG 1917 CA 2064 1973 -1.922 37.648 1.000 16.83 279 1995 ARG ANISOU 1917 CA 279 18.204 84 544 250 ARG 1918 CB MOTA 2609 1897 279 1889 -2.323 37.291 1.000 19.63 ARG ANISOU 1918 CB 279 16.790 233 9 1 1919 CG ARG -63 2196 3139 MOTA 279 2123 -3.288 36.131 1.000 27.03 ANISOU 1919 CG ARG -603 -275 -198 279 16.656 ARG 1920 CD 3150 MOTA 3198 279 3924 -4.578 36.364 1.000 27.45 ANISOU 1920 CD ARG 279 17.236 -359 ARG 1921 NE 2915 MOTA 2854 279 4659 -5.717 36.779 1.000 32.85 ANISOU 1921 NE ARG 279 16.714 1922 CZ ARG MOTA

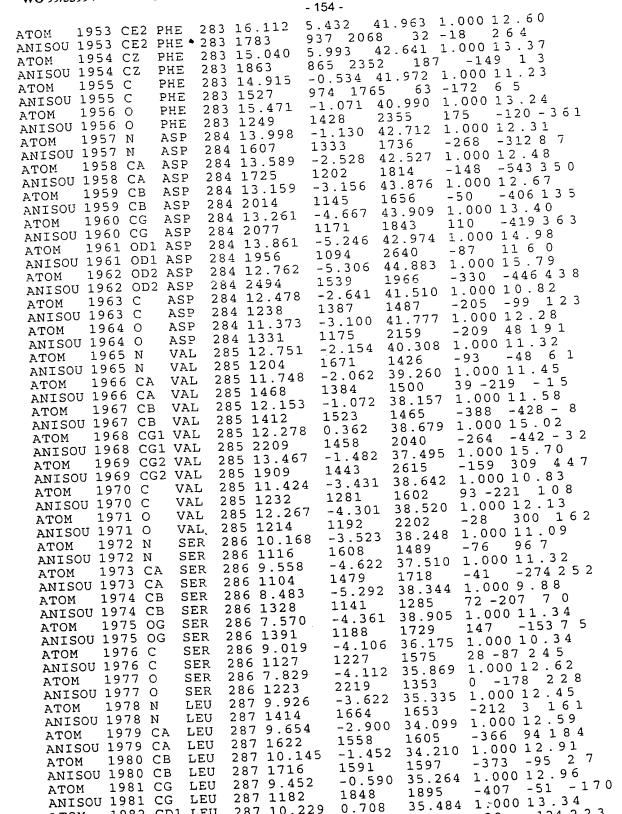


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AION 4302 - 370 A653 2100 4302 - 370 27
ANISOU 1924 NH2 ARG 279 17.551 -6.750 36.890 1.76 3278 -824
ATOM 1924 NH2 ARG 279 4879 2436 7074 1 000 17 48
ANISO 1925 C ARG 279 19.628 -0.519 39.130 75 -8 7 0 5
ATOM 1925 C ARG 279 2118 1653 2071 1 000 26 . 82
1025 O ARG 279 19.916 -1.004 1227 -1467 1383
ANT COLUMN 1926 O ARG 279 3764 31620 30 505 1 000 17.73
rmom 1927 N GLU 280 20.538 0.533 2459 109 609 3 7
ANTSOU 1927 N GLU 280 1983 22 2317 39 026 1.000 19.66
ATOM 1928 CA GLO 200 2110 2023 3396 125 215 /3/
ANTSOU 1928 CA GLU 280 2049 20 20 37 936 1.000 20 . 17
NMOM 1929 CB GLU 200 221.01 3457 3560 464 130 1000
ANTSOU 1929 CB GLU 280 1040
ΔΨΩM 1930 CG GEO - 1 175 447/ 801 110/
ANISOU 1930 CG GLU 280 23 698 0.341 35.590 1.000 13.20 6
ATOM 1931 CD GEO 200 5144 5703 4221 -64 1339 6
ANISOU 1931 CD 320 24 466 1.327 35.685 1.000 574 1639
ANTSOU 1992 OF 280 23 489 -0.294 34.319 1.00 194 1 0 2
ATOM 1023 OF2 GLU 280 5257 6/4/ 3/61 1 000 19 68
ANISO 1934 C GLU 280 21.984 1.188 40.20 1.566 162 4 9 0
ATOM 1934 C GLU 280 1488 2350 3640 1 000 25 . 69
ATOM 1935 O GLU 280 23.031 1.122 4123 231 -245 180
ATOM 1935 O. GLU 280 1871 3/66 412 565 1 000 18.57
20.943 1.300 2.81 1 7 6
ANTSOU 1936 N CYS 281 1560 2 762 41 806 1.000 23.83
ATOM 1937 CA CYS 281 21.096 2547 3184 -1189 176 -122
ANISOU 1937 CA CYS 201 21 079 4 264 41.523 1.000 25.40
ATOM 1938 CB CYS 201 21.0. 3655 3718 -426 300 - 1
ANISOU 1938 CB C13 201 10 507 4 904 40.763 1.000 27.00
ATOM 1939 SG CVC 281 3069 2914 4295 -522 16 99
ANISO 1949 C CVS 281 20.098 2.406 42.507 100 -6 -5 4 6
ATOM 1040 C CYS 281 1377 1604 3473 1 000 17 . 04
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ANISOU 1941 O CYS 281 223 19.447 1.245 42.794 1.000 15.23 ATOM 1942 N GLY 282 19.447 1.597 2572 3 -58 - 436
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ANTSOU 1943 CA GLY 282 1565 0 519 43 727 1.000 13 . / 5
ATOM 1944 C 324 1562 2029 -270 440
ANISOU 1944 C GLY 282 16 585 0 012 44.639 1.000 14.99
ATOM 1945 O GLI 202 1011 1630 2313 207 -242 433
ANISOU 1945 O BUT 203 16 744 1.009 42.582 1.000 12. 252
ATOM 1946 N PHE 283 1434 1803 1570 -200 11 80
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ANTICOU 1947 CA PHE 283 1477 1032 1974 1 000 14 . 13
1948 CB PHE 283 14.839 1.03 109 -187 159
777 1048 CB PHE 283 2262 9/2 2130 757 1 000 12 63
1949 CG PHE 283 14.900 3.332 2055 47 -86 9
ANTSON 1949 CG PHE 283 1/11 1000 13.45
NTOM 1950 CD1 PHE 283 13.631 1222 2013 -166 24 - 229
ANTSON 1950 CD1 PHE 283 1697 1311 41 519 1.000 13.15
ATOM 1951 CD2 PHE 283 16:03/ 1:125 2295 142 -41 -99
ANISOU 1951 CD2 PRE 283 13 903 5.248 42.839 1.000 15.61 7
NTOM 1952 CEL PRE 203 13.203 1640 2171 -202 484 -017
ANISOU 1952 CE1 PHE 283 2111 1649 2171

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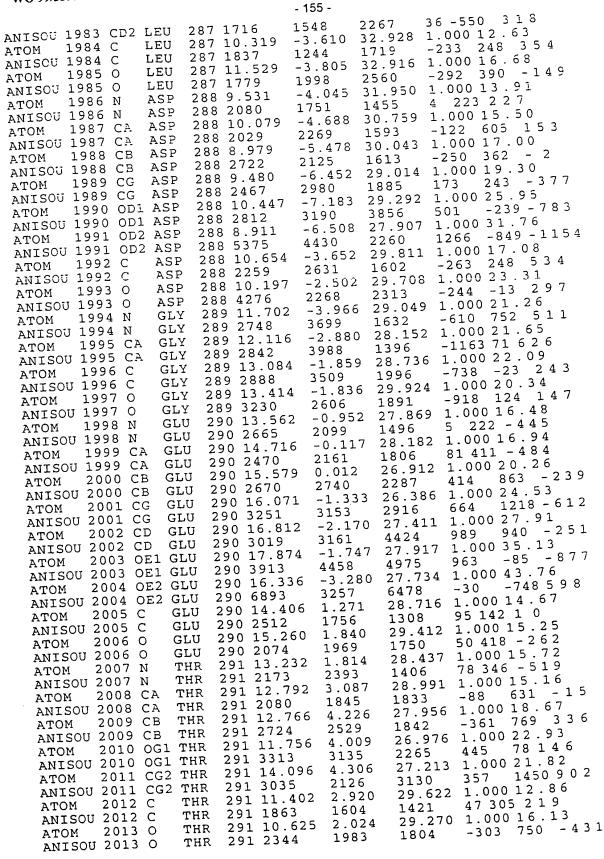
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1983 CD2 LEU

ANISOU 1982 CD1 LEU

MOTA

ATOM



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THR 293 1486 1547
THR 293 7.626 6.715
THR 293 1717 1460
THR 293 6.352 7.215
THR 293 2128 1182 1647 MOTA 32.421 1.000 12.28 ANISOU 2019 N -168 337 -200 2020 CA 1489 MOTA 31.733 1.000 13.27 ANISOU 2020 CA -159 - 284 2021 CB 1730 -258 MOTA 293 2128 31.911 1.000 13.85 THRANISOU 2021 CB 6.237 293 5.317 2022 OG1 THR 8 -131 7 4 2216 1217 30.212 1.000 13.72 293 1831 ANISOU 2022 OG1 THR 7.303 293 6.474 -252 -56 -405 2023 CG2 THR MOTA 1738 293 1791 293 7.363 1683 33.937 1.000 10.58 ANISOU 2023 CG2 THR 6.635 THR 12 447 9 2024 C 1050 1533 ATOM 293 1439 34.553 1.000 10.29 THR ANISOU 2024 C 5.576 293 7.211 -56 93 1 1 8 THR 2025 O 1758 1102 ATOM293 1049 1102 294 7.243 7.810 34.56 1093 1494 293 1049 34.569 1.000 11.53 1494 -307 306 -66 ANISOU 2025 O THR 294 1794 1093 1494 -307 306 -294 6.806 7.939 35.950 1.000 10.41 294 6.806 7.939 35.950 1.000 10.41 294 1432 1061 1463 -174 125 -1 294 6.709 9.426 36.336 1.000 12.25 294 1930 1030 1694 -164 292 -PHE 2026 N MOTA ANISOU 2026 N PHE -174 125 -162 ATOM 2027 CA ANISOU 2027 CA PHE PHE -164 292 -64 PHE2028 CB 294 1930 1030 1694 -164 292 -294 6.270 9.658 37.770 1.000 12.77 294 1880 1136 1837 -103 178 -294 7.123 9.462 38.839 1.000 14.73 294 1976 1893 1727 -539 161 -MOTA ANISOU 2028 CB PHE -103 178 -427 2029 CG PHE MOTA ANISOU 2029 CG PHE -539 161 -132 2030 CD1 PHE MOTA 294 4.989 10.068 38.056 1.000 16.59 ANISOU 2030 CD1 PHE 386 - 492 2031 CD2 PHE 294 2180 1923 294 2180 9 673 2199 ATOM40.144 1.000 14.36 ANISOU 2031 CD2 PHE
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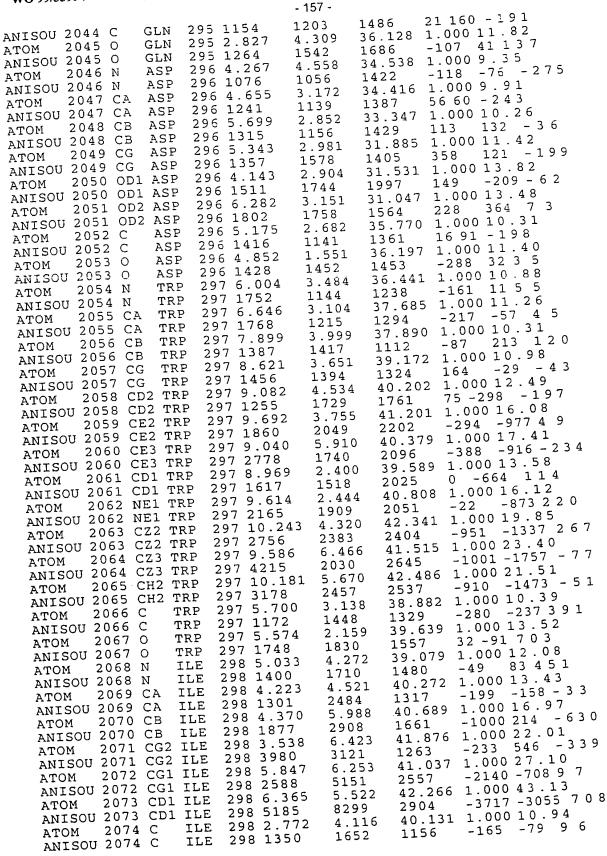
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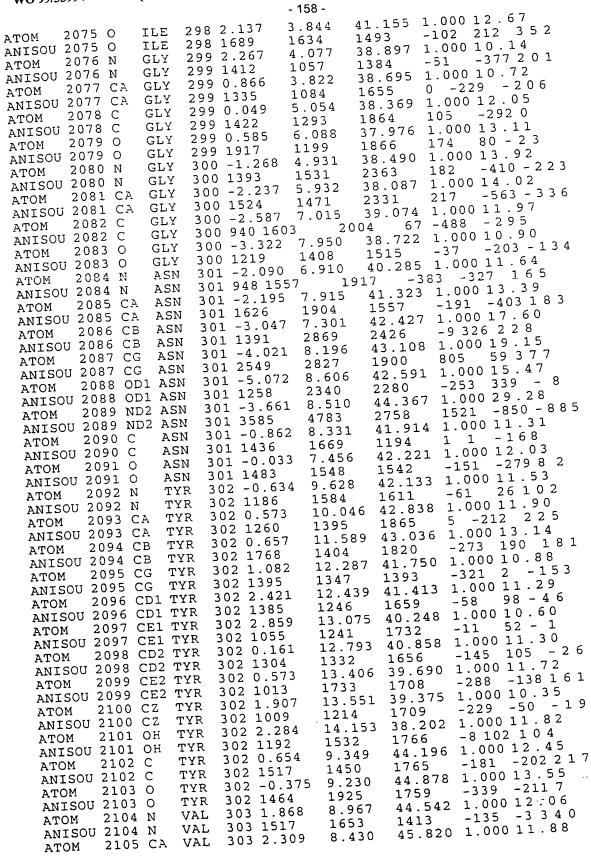
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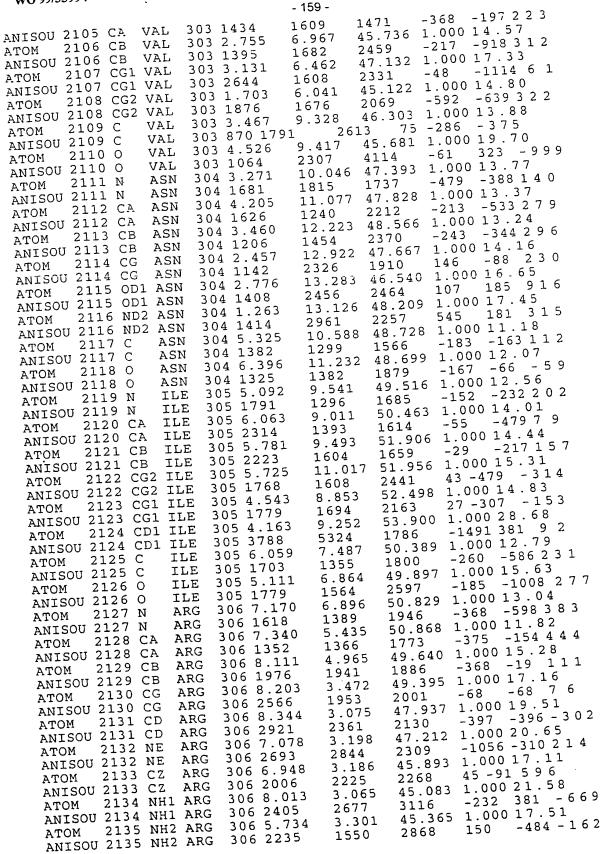
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 -505 280 -118 2032 CE1 PHE MOTA ANISOU 2032 CE1 PHE 144 -602 2033 CE2 PHE MOTA ANISOU 2033 CE2 PHE 97 - 135 2034 CZ PHE MOTA PHE ANISOU 2034 CZ 294 5.484 -155 78 1 3 7 PHE 2035 C MOTA 1536 1200 37.125 1.000 10.67 294 1401 PHE ANISOU 2035 C 6.425 294 5.325 294 1396 PHE 90 337 1 0 5 2036 0 1297 1360 MOTA 35.299 1.000 10.62 PHE ANISOU 2036 O 7.355 295 4.487 88 - 24 2037 N GLN -18 1187 1450 MOTA 35.393 1.000 11.31 295 1399 ANISOU 2037 N GLN 6.612 -96 120 -321 295 3.217 2038 CA GLNMOTA 1660 1205 295 1433 34.254 1.000 11.66 ANISOU 2038 CA GLN7.053 295 2.284 7.053 34.254 1.000 12 -141 295 1425 1053 1953 -25 63 -141 295 1425 1053 2039 CB GLNATOM 295 1425 6.360 34.200 1.000 11.05 1011 1614 -93 -1181 ANISOU 2039 CB GLN -118 1 8 295 0.951 GLN 2040 CG MOTA 295 1573 6.843 33.087 1.000 11.35 GLN ANISOU 2040 CG 295 0.052 57 - 13 2041 CD GLN 173 1326 1395 MOTA 32.378 1.000 15.06 295 1592 ANISOU 2041 CD GLN295 0.349 7.823 2042 OE1 GLN 182,5 - 110 7 MOTA 295 2306 1589 32.914 1.000 13.90 ANISOU 2042 OE1 GLN 295 -1.053 6.153 156 -282 2 0 8 2043 NE2 GLN 295 1511 1757 2015 ATOM . ANISOU 2043 NE2 GLN 35.389 1.000 10.12 5.107 295 3.412 GLN 2044 C ATOM









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		- 160 - 5 . 027	52 155 1	000 13.45
ATOM 2136 C	ARG 306 8.035 ARG 306 2254	1018	1837 -	-246 -481 9 8
ANISOU 2136 C	ARG 306 2254 ARG 306 9.006	5.682	52.556 1	1.000 12.15
ATOM 2137 O	ARG 306 1902	1099		-18 -362 - 8 0
ANISOU 2137 O ATOM 2138 N	ARG 307 7.571	3.968		1.000 18.19 -734 -938 7 9 2
ATOM 2138 N ANISOU 2138 N	ARG 307 3073	1620	2218 · 53.989 :	1.000 19.20
ATOM 2139 CA	ARG 307 8.197	3.380	2277	-675 -1236 643
ANISOU 2139 CA	ARG 307 3053	1963 2.191	53 611	1 000 23.08
ATOM 2140 C	ARG 307 9.086 ARG 307 4018		2847	-270 -1885 3 ^{2 9}
ANISOU 2140 C ATOM 2141 O	ARG 307 4018 ARG 307 8.636	1.292		1.000 35.93
ATOM 2141 0 ANISOU 2141 0	ARG 307 6003	2403		38 -3227 - 791 1.000 28.25
ATOM 2142 CB	ARG 307 7.131	2.918	54.997 1882	-1503 -277 5 0 9
ANTSOU 2142 CB	ARG 307 5557		55.275	1.000 33.39
ATOM 2143 CG	ARG 307 6.032 ARG 307 4564		3261	-1613 731 208
ANISOU 2143 CG ATOM 2144 CD			56.317	1.000 40.42
ATOM 2144 CD ANISOU 2144 CD		5701	3322	-1900 1263 9 7 1 1.000 50.83
ATOM 2145 NE	ARG 307 5.605	2.952	57.529	-2786 105 1 6 2 4
ANTSOU 2145 NE	ARG 307 8119	7287	3908 58.530	1 000 51.36
ATOM 2146 CZ	ARG 30/4.894	2.441 8064		-3650 -966 2451
ANISOU 2146 CZ	ARG 307 7424 1 ARG 307 3.567		58.485	1 000 69.51
ATOM 2147 NH ANISOU 2147 NH		10951	7874	-6970 -2008 3 2 4 3
ATOM 2148 NH	2 ARG 307 5.489	9 1.937	59.600	
ANISOU 2148 NH	12 ARG 307 1071	8150	3930	1.000 22.92
ATOM 2149 N	THR 308 10.3	47 2.147 2587		-589 -200 I / C
ANISOU 2149 N	THR 308 2759 THR 308 11.2		53.794	1.000 24.47
ATOM 2150 CA ANISOU 2150 CA		2649	3268	-360 52 1 5 0
ATOM 2151 C	THR 308 10.6	02 -0.25	254.382 4044	1.000 31.10 -768 16 2 7 9
ANISOU 2151 C	THR 308 5251	2520 10 -1.29		1.000 31.44
ATOM 2152 O	THR 308 10.6 THR 308 4573			-457 -1745 - 40
ANISOU 2152 O ATOM 2153 C		15 1.279	54.378	1.000 23.51 413 -694 5 4 2
ATOM 2153 C ANISOU 2153 C	B THR 308 3718	2086	3131	
атом 2154 О	G1 THK 308 13.1	95 2.410		153 437 - 9
ANISOU 2154 O	G1 THR 308 2711 G2 THR 308 13.5	L 2503 573 0.141	54.117	7 1.000 26.37
ATOM 2155 C ANISOU 2155 C		7 2796	2796	927 -329 - 10
AN1SOU 2155 C ATOM 2156 N	SER 309 10.0	066 -0.15	6 55.59	6 1.000 28.39 -19 2 1300
ANISOU 2156 N	SER 309 375	9 2774 88 -1.33	4252 35 56.23	0 1 000 34 . 69
ATOM 2157 C	A SER 309 9.4		3925	-1066 -1089 1626
ANISOU 2157 C			37 55.72	4 1.000 41.41
ATOM 2158 (ANISOU 2158 (SER 309 644	2 3910	5383	-2171 -1170 2144 2 1.000 57.05
ATOM 2159	SER 309 7.6	72 -2.8		-4907 -2077 2027
ANISOU 2159	O SER 309 113	89 5141 50 -1.1		5 1 000 31.61
ATOM 2160	CB SER 309 9.4 CB SER 309 486		4188	-483 368 962
ANISOU 2160 ATOM 2161		85 -0.1	35 58.10)7 1.000 38.99 313 -2249 -496
ANISOU 2161	OG SER 309 473	31 3477	6604 68 55.03	22 1 000 47 . 69
ATOM 2162	N FAS 310 \.	391 -0.8 02 5577		-539 -1369 1583
ANISOU 2162	N LYS 310 550 FE IUM 312 8.5		166 54.05	55 1.000 11.05
ATOM 2163 ANISOU 2163	• =	90 1156	1351	-101 -23//1
ATOM 2164	C1 AKG 313 5.	987 14.8	315 54.6	
ANISOU 2164	C1 AKG 313 27	77 2119 799 15.3	2572 240 54.6	59 1.000 20 .82
ATOM 2165	01 AKG 313 4.		3 2659	514 -234 2 6 4
ANISOU 2165 ATOM 2166		•		87 1.000 17.79
ATOM 2166	04 ANG 313 0.			



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WU 99/3	3774		$\overline{}$			161 -		
ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU ATOM ANISOU	2166 2167 2167 2168 2168 2169 2169 2170 2170 2171		AKG AKG AKG AKG AKG AKG AKG AKG AKG	313 313 313 313 313 313 313 313	3246 6.923 3122	-161 - 1765 15.178 2566 14.661 2066 16.080 1910 16.741 1761 17.816 1840 18.591	2587 55.844 3068 55.821 2334 56.872 3581 57.716 3160 58.672 3618 59.124	74 -377 429 1.000 20.08 -528 419 -399 1.000 17.60 -314 226 -252 1.000 21.69 240 62 -327 1.000 21.50 199 -143 -185 1.000 22.58 755 -495 -313 1.000 27.48
ATOM ANISOU ATOM ANISOU	2172 2173	03 04	AKG AKG AKG	313 313	3581 5.660 3191	2470 17.889 2809	4389 58.999 4846	-34 602 -1266 1.000 28.55 612 -246 -1148
ATOM ATOM	2174 2175	S 01	SO4	401	11.676 11.293 12.501	0.439 0.826 -0.829	24.942 26.321 25.014	1.000 40.14 1.000 33.12 1.000 35.79
ATOM ATOM ATOM	2176 2177 2178	03	SO4 SO4	401		0.189	24.129 24.329	1.000 54.89
ATOM MOTA MOTA	2179 2180	OW	нон нон	501 502	6.455 ! -10.52	10.219 18.612	50.560	1.000 12.86
ATOM ATOM	2181 2182	. OW	нон нон	503 504	3 - 8.644 $1 - 10.31$		43.074	1.000 16.10

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536 27.068

537 13.523

540 -1.548

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524 -15.683 28.618 525 -5.386 20.413

533 -12.450 16.848

519 -14.415

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506 -6.873

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ATOM	2220 OW HOH 542 15.389 11.536 32.065 1.000 1	7.88
ATOM	2221 OW HOH 543 18.496 6.995 52.191 1.000 J	. / . 4 /
ATOM	2222 ON HOH 544 19 848 22.580 35.334 1.000 J	7.28
MOTA	2223 OW HOH 545 -0.387 4.787 41.967 1.000	13.22
MOTA	2224 OW HOH 546 23.502 12.662 35.308 1.000	18.14
ATOM	2225 OW HOH 547 10.332 25.236 33.926 1.000	19.05
ATOM	2226 OW HOH 548 21.447 20.605 34.090 1.000	1 / . 2 4
ATOM	2227 OW HOH 549 8.164 7.685 27.077 1.000	25.40
ATOM	2228 OW HOH 550 14.393 -5.127 40.321 1.000	15.00
ATOM	2229 OW HOH 551 12.873 29.356 39.662 1.000	10.45
ATOM	2230 OW HOH 552 11.974 24.144 58.426 1.000	19.71
ATOM	2231 OW HOR 555 17.521 7.545 1.000	23.76
MOTA	2232 OW HOR 534 3.401 2.031	18.44
ATOM	2233 OW HOR 555 10.005 20.017 1 000	19.57
ATOM	2234 OW HOR 330 10.027 12.070 66 466 1 000	20.84
ATOM	2235 OW HOR 337 20:030 10:000	21.62
MOTA	2236 OW HOR 330 11.313 20.516 43 046 1 000	16.22
MOTA	2237 0W ROR 560 2 616 15 488 32 365 1 000	19.40
\mathtt{MOTA}	2238 OW ROR 501 3.000 4.903 27.857 1.000	22.74
MOTA	2239 OW HOR 561 31.000	22.98
ATOM	2240 OW HON 502 20.430 1.000	26.36
ATOM	2241 00 1001 564 18 595 6 141 37 697 1.000	25.10
MOTA MOTA	2243 OM HOH 565 22 446 13.893 31.420 1.000	29.00
ATOM	2244 OW HOH 566 6 586 3.577 28.350 1.000	27.82
MOTA	2245 OW HOH 567 6.250 20.077 30.961 1.000	23.27
ATOM	2246 OW HOH 568 7.341 16.113 31.186 1.000	28.59
ATOM	1 2247 OW HOH 569 16.090 32.070 42.552 1.000	25.17
ATOM	1 2248 OW HOH 570 11.500 28.800 57.501 1.000	28.58
MOTA	1 2249 OW HOH 571 12.901 26.768 58.391 1.000	28.82
MOTA	4 2250 OW HOR 5/2 -1/.5/1 27 100 1 000	39.05
\mathtt{MOTA}	4 2251 OW ROR 573 23.202 26 440 51 734 1.000	29.03
MOTA	4 2252 OW ROR 575 1 199 19 088 42 527 1.000	14.86
MOTA	M 2253 0W NON 575 4 389 33 026 63 392 1.000	29.56
ATOM	2055 0W HOW 577 17 569 25 732 32 249 1.000	20.62
MOTA MOTA	2255 OW HOH 578 -19.107 12.822 67.516 1.000	22.35
ATOM	M 2257 OW HOH 579 29.333 19.198 51.975 1.000	22.51
MOTA	2258 OW HOH 580 27.950 27.635 51.903 1.000	25.40
MOTA	M 2259 OW HOH 581 -21.085 14.501 68.535 1.000	21.19
MOTA	M 2260 OW HOH 582 1.529 17.378 33.953 1.000) 25.29) 33.92
ATOM	M 2261 OW HOH 583 9.138 20.887 66.894 1.00	0 17.48
MOTA	M 2262 OW HOR 304 - 11:03 12 507 42 347 1 00	0 2 2 . 0 9
ATOM	M 2203 0W 11011 505 1.7 762 31 369 39 046 1 00	0 20 . 79
ATOM	M 2284 OW HOR 500 11, 500 25 439 41 729 1 00	0 29 . 68
MOTA	M 2265 0W ROT 500 7 877 1 046 29 689 1.00	0 27 . 70
MOTA	om 2200 ow non 500 27 995 13 540 42 235 1.00	0 25 . 9 1
MOTA	om 2267 ov von 500 1 276 14 852 34 021 1.00	020.41
ATOM	2262 21 124 522 24 179 41 242 1.00	0 26 . 77
ATOM ATOM	2270 OW HOH 592 0.404 14.096 36.006 1.00	0 27 . 9 2
ATOM	2271 OW HOH 593 -2.835 36.981 57.827 1.00	0 31 . 86
ATOM	OM 2272 OW HOH 594 3.276 0.788 39.940 1.00	0 32 . 07
ATOM	OM 2273 OW HOH 595 11.025 -8.794 31.468 1.00	0 27 . 18
ATOM	OM 2274 OW HOH 596 6.301 2.276 42.639 1.00	0 43.75
ATOM	OM 2275 OW HOH 597 29.302 16.146 62.924 1.00	0 3 0 . 8 5
MOTA	OM 22/6 OW HOR 398 13:033 20:000 C4 519 1 00	0 4 2 . 6 2
ATON	OM 2277 OW NOT 600 31 480 10 826 34 742 1.00	00 25 . 74
ATON	OM 2278 OW HOR 600 21.400 10.010 18.566 1.00	0030.92
ATO	OM 2279 OW HOR 601 2,000 20 841 43 352 1 0	00 43.96
IOTA	OM 2280 OW HOH 602 -3.928 29.841 43.352 1.0	

- 162 -



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WO 99/33994
                                  - 163 -
                                         34.437 1.000 33.10
                                  21.563
                     603 2.885
                                          25.270 1.000 38.18
                HOH
       2281 OW
ATOM
                                  6.043
                     604 11.801
                нон
                                                 1.000 18.48
       2282 OW
                                          40.472
MOTA
                                  17.197
                     605 -1.019
       2283 OW
                HOH
                                                 1.000 22.54
                                          68.110
MOTA
                                  23.349
                     606 18.382
       2284 OW
                HOH
                                                  1.000 17.64
                                          45.609
ATOM
                                  8.137
                     607 -8.141
                HOH
                                                  1.000 24.29
       2285 OW
ATOM
                                          51.700
                                  2.667
                      608 5.022
                HOH
       2286 OW
                                                  1.000 21.94
                                          33.490
MOTA
                      609 17.557
                                  10.755
                нон
                                                 1.000 20.61
       2287 OW
ATOM
                                          49.675
                                  1.201
                      610 11.222
                                          50.509 1.000 22.18
                HOH
       2288 OW
ATOM
                                  35.047
                      611 4.243
                                          56.082 1.000 22.08
                HOH
       2289 OW
ATOM
                                  4.031
                      612 11.103
                                          36.791 1.000 32.32
                HOH
       2290 OW
                      613 11.366 31.522
614 -21.189 24.787
ATOM
                                          52.739 1.000 31.83
       2291 OW
                нон
MOTA
                                          30.674 1.000 24.77
       2292 OW
                 HOH
ATOM
                                  -1.491
                      615 7.847
                                          31.445 1.000 25.97
       2293 OW
                 HOH
ATOM
                      616 19.041
                                  11.937
                                          40.410 1.000 29.24
                 HOH
        2294 OW
ATOM
                                   29.879
                      617 6.221
                                           35.280 1.000 23.72
                 HOH
        2295 OW
MOTA
                      618 17.266
                                  5.933
                                   -7.215 28.510 1.000 28.19
                 HOH
        2296 OW
MOTA
                      619 5.983
                                           57.639 1.000 30.97
        2297 OW
                 HOH
 ATOM
                                   8.129
                      620 22.574
                                                   1.000 28.77
                 HOH
        2298 OW
                                           60.287
 MOTA
                                   7.806
                      621 2.553
                                                  1.000 34.00
                 HOH
        2299 OW
                                  25.812 51.234
 ATOM
                      622 29.939
                 HOH
                                                   1.000 25.88
        2300 OW
                                   34.823 53.632
 MOTA
                      623 2.205
                 HOH
                                                   1.000 28.46
        2301 OW
                                   13.838 67.343
 MOTA
                       624 18.091
        2302 OW
                 HOH
                                                   1.000 26.84
                                           58.475
 ATOM
                                   3.195
                       625 8.342
                                                   1.000 31.11
        2303 OW
                 HOH
                                           42.790
 ATOM
                       626 -16.086 18.427
                                                   1.000 27.48
        2304 OW
                 HOH
 ATOM
                                           35.620
                       627 -2.098 13.445
                                                   1.000 32.55
        2305 OW
                  HOH
 ATOM
                                           42.834
                                   30.471
                       628 0.481
                                                   1.000 28.70
                  HOH
        2306 OW
 ATOM
                                           42.899
                                    33.845
                       629 13.368
                  HOH
                                                   1.000 25.58
         2307 OW
 ATOM
                                           51.533
                       630 -13.792 14.642
                                            29.242 1.000 39.62
                  HOH
         2308 OW
 ATOM
                                    1.461
                       631 3.299
         2309 OW
                  HOH
                                                   1.000 27.75
                                           46.705
 MOTA
                       632 -16.012 20.690
                                                    1.000 27.02
         2310 OW
                  HOH
                                            31.259
 ATOM
                       633 19.606 8.142
         2311 OW
                  HOH
                                                   1.000 30.59
  ATOM
                                            57.205
                                    7.954
                       634 5.077
                                                   1.000 35.68
                  HOH
         2312 OW
  MOTA
                                            45.877
                                   6.963
                       635 -1.502
                                            38.804 1.000 21.84
                  HOH
         2313 OW
  MOTA
                                    17.449
                       636 9.974
         2314 OW
                  HOH
                                            67.228 1.000 25.04
  MOTA
                       637 -22.829 12.836
                                            39.722 1.000 25.88
                  HOH
         2315 OW
  MOTA
                                    34.333
19.798
                        638 6.275
                                            56..051 1.000 26.67
         2316 OW
                  HOH
  MOTA
                        639 2.248
                                            67.454 1.000 31.34
         2317 OW
                  HOH
  ATOM
                        640 -20.552 17.013
                                            28.911 1.000 29.96
                  HOH
         2318 OW
  ATOM
                                    16.570
                        641 9.298
                                            60.074 1.000 28.13
                   HOH
         2319 OW
  MOTA
                                    11.113
                        642 -1.732
                   нон
                                                    1.000 36.36
         2320 OW
                                            44.657
  MOTA
                                     23.604
                        643 34.157
                                            33.576 1.000 34.90
         2321 OW
                   HOH
  ATOM
                                    20.199
                        644 24.298
                                             31.570 1.000 32.66
29.009 1.000 34.61
                   HOH
          2322 OW
  MOTA
                                    -4.667
                        645 13.803
                   HOH
          2323 OW
  ATOM
                                            29.009
                                     -2.594
                        646 6.295
          2324 OW
                   HOH
                                                    1.000 28.08
   MOTA
                                            49.318
                                     37.039
                        647 5.623
                   HOH
                                                    1.000 38.32
          2325 OW
   MOTA
                                            46.868
                        648 -18.805 19.286
                                                    1.000 34.45
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HOH

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2326 OW

2327 OW

2328 OW

2329 OW

2330 OW

2331 OW

2332 OW

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2334 OW

2335 OW

2336 OW

2337 OW

2338 OW

2339 OW

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2341 OW

ATOM

ATOM

ATOM

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MOTA

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MOTA

MOTA

MOTA

649 16.026 35.829

650 -12.187 28.769

653 -14.568 18.811

658 -11.834 15.408

2.125

26.254

13.542

14.669

14.477

38.273

13.918

14.508

33.651

21.602

651 21.344 5.778

652 -1.848

654 -8.655

655 18.836

656 16.217

657 28.678

659 -1.317

661 -3.058

662 10.968

663 28.960

660 8.784

49.382

25.619

38.043

53.330

59.599

28.681

47.405

38.533

53.665

45.330 1.000 27.36

55.101 1.000 27.43

32.240 1.000 32.02

55.775 1.000 29.95

38.301 1.000 32.07

28.102 1.000 32.24

1.000 33.35

1.000 30.94

1.000 33.25

1.000 34.45

1.000 33.62

1.000 28.79

1.000 36.21

1.000 29.25



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ATOM	2342 OW	нон	664 -10.709 26.808 39.175 1.000 42.71
MOTA	2343 OW	HOH	665 17.790 7.093 55.023 1.000 30.29
ATOM	2344 OW	HOH	666 6.404 24.865 29.848 1.000 34.55
MOTA	2345 OW	HOH	667 -15.418 19.777 58.341 1.000 33.82
ATOM	2346 OW	HOH	668 0.000 0.000 37.259 0.330 49.90
ATOM	2347 OW	нон	669 19.652 24.610 33.660 1.000 31.77 670 17 188 9.619 29.950 1.000 29.94
ATOM	2348 OW	нон	070 17.100
ATOM	2349 OW	нон	0/1 1/./00 2.300
MOTA	2350 OW	нон	0/2 = 0.035 3.032 3.032 1 000 00 50
MOTA	2351 OW	нон	0/3 25.037 20.523 00.20
ATOM	2352 OW	нон	0/4 13.433 32.000
MOTA	2353 OW	нон	0/5 -12.040 21.020 0=
ATOM	2354 OW	нон	070 10.233 33.000
\mathtt{ATOM}	2355 OW	нон	0// 5.521 23:322 1 000 40 00
MOTA	2356 OW	НОН	0,0 0.023
ATOM	2357 OW	нон	679 35.052 23.156 52.356 1.000 40.17 680 -12.008 38.355 51.601 1.000 35.18
ATOM	2358 OW	нон	680 -12.008 38.333 31.331 1.330 35.17
ATOM	2359 OW	НОН	682 1.379 2.075 27.532 1.000 46.38
ATOM	2360 OW	HOH HOH	683 -0.516 -2.480 37.686 1.000 21.77
ATOM	2361 OW 2362 OW	нон	684 4.567 10.310 43.503 1.000 24.86
MOTA	2362 OW 2363 OW	нон	685 19.443 5.558 61.133 1.000 36.06
MOTA	2364 OW	нон	686 3 205 29.499 40.656 1.000 36.99
ATOM ATOM	2365 OW	нон	687 32 498 16.774 43.447 1.000 41.18
ATOM	2366 OW	нон	688 28 166 23.113 57.593 1.000 35.56
ATOM	2367 OW	нон	689 -17 023 23 220 46 759 1 000 30 05
ATOM	2368 OW	нон	690 15 567 7.782 28.910 1.000 32.51
ATOM	2369 OW		691 11 780 30.287 57.203 1.000 33.34
ATOM	2370 OW		692 24 449 12.699 32.400 1.000 34.99
ATOM	2371 OW		693 26.200 25.005 57.918 1.000 39.38